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APPLICATION

for

UNITED STATES LETTERS PATENT

on

1,2-DISUBSTITUTED-6-OXO-3-PHENYL-PIPERIDINE-3-CARBOXAMIDES  
AND COMBINATORIAL LIBRARIES THEREOF

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## **1,2-DISUBSTITUTED-6-OXO-3-PHENYL-PIPERIDINE-3-CARBOXAMIDES.**

### **AND COMBINATORIAL LIBRARIES THEREOF**

#### **FIELD OF THE INVENTION**

**[0001]** The present invention relates generally to the synthesis of compounds comprising piperidine-3-carboxamides. In one embodiment, the invention provides novel 1,2-disubstituted-6-oxo-3-phenyl-piperidine-3-carboxamide derivative compounds as well as novel combinatorial libraries comprised of such compounds.

#### **BACKGROUND INFORMATION**

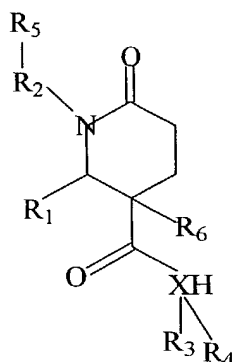
**[0002]** The process of discovering new therapeutically active compounds for a given indication involves the screening of all compounds from available compound collections. From the compounds tested, one or more structures are selected as a promising lead. A large number of related analogs are then synthesized in order to develop a structure-activity relationship and select one or more optimal compounds. With traditional "one-at-a-time" synthesis and biological testing of analogs, this optimization process is long and labor intensive. Adding significant numbers of new structures to the compound collections used in the initial screening step of the discovery and optimization process cannot be accomplished with traditional "one-at-a-time" synthesis methods, except over a time frame of years or even decades. Faster methods are needed that allow for the preparation of up to thousands of related compounds in a matter of days or a few weeks. This need is particularly evident when it comes to synthesizing more complex compounds, such as piperidine-3-carboxamide derivative compounds.

**[0003]** Combinatorial approaches have been extended to "organic," or non-peptide, libraries. However, the libraries to date contain compounds of limited



## SUMMARY OF THE INVENTION

**[0006]** The present invention relates to novel piperidine-3-carboxamide derivative compounds of the following formula:



wherein

**[0007]** X is selected from the group consisting of N and O;

**[0008]** R<sub>1</sub> is selected from the group consisting of a substituted aromatic heterocyclic ring, C<sub>3</sub>-C<sub>12</sub> substituted alicycle and substituted phenyl;

**[0009]** R<sub>2</sub> is selected from the group consisting of H; -OH; C<sub>1</sub> to C<sub>7</sub> alkoxy; C<sub>1</sub> to C<sub>7</sub> substituted alkoxy; C<sub>2</sub>-C<sub>7</sub> alkenyl; C<sub>1</sub> to C<sub>7</sub> substituted alkenyl; C<sub>2</sub> to C<sub>7</sub> alkynyl; C<sub>2</sub> to C<sub>7</sub> substituted alkynyl; unsubstituted phenyl; naphthyl; substituted phenoxy; C<sub>2</sub> to C<sub>7</sub> heterocyclic ring; substituted C<sub>2</sub> to C<sub>7</sub> heterocyclic ring; substituted cyclic C<sub>2</sub> to C<sub>7</sub> alkylene; C<sub>1</sub> to C<sub>7</sub> alkyl; C<sub>1</sub> to C<sub>7</sub> substituted alkyl; C<sub>3</sub> to C<sub>7</sub> cycloalkyl; C<sub>3</sub> to C<sub>7</sub> substituted cycloalkyl; C<sub>1</sub> to C<sub>7</sub> alkoxy; halo; C<sub>1</sub> to C<sub>10</sub> alkylthio; C<sub>1</sub> to C<sub>10</sub> substituted alkylthio; C<sub>1</sub> to C<sub>10</sub> alkyl nitrile; a C<sub>7</sub> to C<sub>18</sub> substituted phenylalkyl; substituted phenyl;

**[0010]** R<sub>3</sub> and R<sub>4</sub> are independently selected from the group consisting of -OH; H; C<sub>1</sub> to C<sub>6</sub> alkyl; C<sub>1</sub> to C<sub>7</sub> substituted alkyl; C<sub>2</sub> to C<sub>7</sub> alkenyl; C<sub>1</sub> to C<sub>7</sub> alkoxy; C<sub>1</sub> to C<sub>7</sub> substituted alkoxy; C<sub>3</sub> to C<sub>7</sub> cycloalkyl; C<sub>3</sub> to C<sub>7</sub> substituted cycloalkyl; C<sub>1</sub>

to C<sub>10</sub> alkylthio; C<sub>1</sub> to C<sub>10</sub> alkyl nitrile; C<sub>1</sub> to C<sub>4</sub> alcohol; substituted phenyl; C<sub>1</sub> to C<sub>6</sub> substituted alkyl; C<sub>1</sub> to C<sub>7</sub> alkoxy; C<sub>3</sub> to C<sub>7</sub> cycloalkyl; and C<sub>3</sub> to C<sub>7</sub> substituted cycloalkyl; C<sub>2</sub> to C<sub>7</sub> heterocyclic ring; C<sub>2</sub> to C<sub>7</sub> substituted heterocyclic ring; phenoxy; and substituted phenoxy,

**[0011]** R<sub>5</sub> is selected from the group consisting of H and NH<sub>2</sub>, and

**[0012]** R<sub>6</sub> is selected from the group consisting of phenyl, substituted phenyl, C<sub>2</sub> to C<sub>7</sub> heterocyclic ring, and substituted C<sub>2</sub> to C<sub>7</sub> heterocyclic ring.

**[0013]** The invention further relates to combinatorial libraries containing two or more such compounds, as well as methods of preparing piperidine-3-carboxamide derivative compounds.

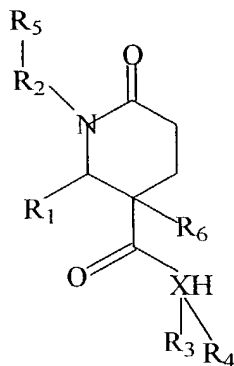
#### BRIEF DESCRIPTION OF THE DRAWING

**[0014]** Figures 1 and 2 show two parts of a scheme for the combinatorial synthesis of piperidine-3-carboxamide derivative compounds.

**[0015]** Figure 3 shows a scheme for the production of (Substituted Phenyl)-glutaric anhydrides.

#### DETAILED DESCRIPTION OF THE INVENTION

**[0016]** The present invention provides compounds and combinatorial libraries of compounds of the formula:



wherein:

**[0017]** X is selected from the group consisting of N and O;

**[0018]** R<sub>1</sub> is selected from the group consisting of a substituted aromatic heterocyclic ring, C<sub>3</sub>-C<sub>12</sub> substituted alicycle and substituted phenyl;

**[0019]** R<sub>2</sub> is selected from the group consisting of H; -OH; C<sub>1</sub> to C<sub>7</sub> alkoxy; C<sub>1</sub> to C<sub>7</sub> substituted alkoxy; C<sub>2</sub>-C<sub>7</sub> alkenyl; C<sub>1</sub> to C<sub>7</sub> substituted alkenyl; C<sub>2</sub> to C<sub>7</sub> alkynyl; C<sub>2</sub> to C<sub>7</sub> substituted alkynyl; unsubstituted phenyl; naphthyl; substituted phenoxy; C<sub>2</sub> to C<sub>7</sub> heterocyclic ring; substituted C<sub>2</sub> to C<sub>7</sub> heterocyclic ring; substituted cyclic C<sub>2</sub> to C<sub>7</sub> alkylene; C<sub>1</sub> to C<sub>7</sub> alkyl; C<sub>1</sub> to C<sub>7</sub> substituted alkyl; C<sub>3</sub> to C<sub>7</sub> cycloalkyl; C<sub>3</sub> to C<sub>7</sub> substituted cycloalkyl; C<sub>1</sub> to C<sub>7</sub> alkoxy; halo; C<sub>1</sub> to C<sub>10</sub> alkylthio; C<sub>1</sub> to C<sub>10</sub> substituted alkylthio; C<sub>1</sub> to C<sub>10</sub> alkyl nitrile; a C<sub>7</sub> to C<sub>18</sub> substituted phenylalkyl; substituted phenyl;

**[0020]** R<sub>3</sub> and R<sub>4</sub> are independently selected from the group consisting of -OH; H; C<sub>1</sub> to C<sub>6</sub> alkyl; C<sub>1</sub> to C<sub>7</sub> substituted alkyl; C<sub>2</sub> to C<sub>7</sub> alkenyl; C<sub>1</sub> to C<sub>7</sub> alkoxy; C<sub>1</sub> to C<sub>7</sub> substituted alkoxy; C<sub>3</sub> to C<sub>7</sub> cycloalkyl; C<sub>3</sub> to C<sub>7</sub> substituted cycloalkyl; C<sub>1</sub> to C<sub>10</sub> alkylthio; C<sub>1</sub> to C<sub>10</sub> alkyl nitrile; C<sub>1</sub> to C<sub>4</sub> alcohol; substituted phenyl; C<sub>1</sub> to C<sub>6</sub> substituted alkyl; C<sub>1</sub> to C<sub>7</sub> alkoxy; C<sub>3</sub> to C<sub>7</sub> cycloalkyl; and C<sub>3</sub> to C<sub>7</sub> substituted cycloalkyl; C<sub>2</sub> to C<sub>7</sub> heterocyclic ring; C<sub>2</sub> to C<sub>7</sub> substituted heterocyclic ring; phenoxy; and substituted phenoxy,

**[0021]** R<sub>5</sub> is selected from the group consisting of H and NH<sub>2</sub>, and

**[0022]** R<sub>6</sub> is selected from the group consisting of phenyl, substituted phenyl, C<sub>2</sub> to C<sub>7</sub> heterocyclic ring, and substituted C<sub>2</sub> to C<sub>7</sub> heterocyclic ring.

**[0023]** The invention also provides methods of preparing piperidine-3-carboxamide derivative compounds and combinatorial libraries. In one method, as shown in Figures 1 and 2, such compounds can be prepared by a process comprising:

**[0024]** preparing a resin bound aldehyde or diamine,

**[0025]** reacting said resin bound aldehyde with an amine, or said resin bound diamine with an aldehyde, to form a resin bound imine,

**[0026]** cyclizing said resin bound imine to produce a resin bound carboxylic acid,

**[0027]** acylating said resin bound carboxylic acid, and

**[0028]** cleaving and extracting said piperidine-3-carboxamide derivative compound from said resin.

**[0029]** Examples of aldehydes which are useful in the above reaction include but are not limited to 4-hydroxybenzaldehyde, 3-hydroxybenzaldehyde, 2-hydroxy-5-methylbenzaldehyde, 3,5-dimethyl-4-hydroxybenzaldehyde, 2-hydroxy-4-methoxybenzaldehyde, 3-ethoxysalicylaldehyde, 2-hydroxy-1-naphthaldehyde, 5-bromosalicylaldehyde, cyclopropanecarboxaldehyde, 3-furaldehyde, benzaldehyde, 2-thiophenecarboxaldehyde, 3-thiophenecarboxaldehyde, P-tolualdehyde, 4,5-dimethyl-2-furancarboxaldehyde, P-anisaldehyde, 5-methylfurfural, O-tolualdehyde, 2,4,5-trimethylbenzaldehyde, piperonal, 5-methyl-2-thiophenecarboxaldehyde, 4-(difluoromethoxy)benzaldehyde, 5-bromo-2-furaldehyde, 4-biphenylcarboxaldehyde and 5-bromo-2-thiophenecarboxaldehyde.

**[0030]** Examples of diamines and amines useful in the above reaction when producing a resin bound diamine or reaction an aldehyde with an amine, include but are not limited to methylamine, ethylamine, propargylamine, cyclopropylamine, allylamine, propylamine, 3-aminopropionitrile, isobutylamine, cyclopentylamine, cyclohexylamine, hexylamine, N-acetylenediamine, 3-ethoxypropylamine, 4-chlorobenzylamine, 1-(3-aminopropyl)-2-pyrrolidinone, tryptamine, 3-(trifluoromethyl)benzylamine, 2,4-dichlorophenethylamine, 4-amino-1-benzylpiperidine, benzylamine, ethylenediamine, 1,3-diaminopropane, 1,4-diaminobutane, trans-1,2-cyclohexanediamine, trans-1,4-diaminocyclohexane, 2,2-thiobis(ethylamine), and N,N-Bis(3-aminopropyl)methylamine.

**[0031]** Examples of amines useful in the above reaction when acylating the resin bound carboxylic acid include but are not limited to nipecotamide, 1-(2-aminoethyl)pyrrolidine, pyrrolidine, histamine, cyclopentylamine, allylamine, 2-methoxyethylamine, cyclohexylamine, 1-methylpiperazine, tetrahydrofurfurylamine, 4-methylbenzylamine, 3-fluorobenzylamine, 4-fluorobenzylamine, 1-(3-aminopropyl)imidazole, cyclopropylamine, propylamine, ethanolamine, 2-thiophenemethylamine, n,n-dimethyl-1,3-propanediamine, 1-(2-

aminoethyl)piperidine, isoamylamine, 3-ethoxypropylamine, (r)-(-)-1-cyclohexylethylamine, neopentylamine, 3-(methylthio)propylamine, isobutylamine, 3-amino-1-propanol, 2-ethoxyethylamine, 2,6-dimethylpiperazine, propargylamine, thiophene-2-ethylamine, butylamine, 2-amino-1-methoxypropane, 3-aminopropionitrile, 3-methylpiperidine, P-anisidine, 1,2,3,6-tetrahydropyridine, 2,6-dimethylmorpholine, methoxyamine hydrochloride, n-ethylpiperazine, water, and hydroxylamine.

**[0032]** When the above-described compounds include one or more chiral centers, the stereochemistry of such chiral centers can independently be in the R or S configuration, or a mixture of the two. The chiral centers can be further designated as R or S or R,S or d,D, l,L or d,l, D,L.

**[0033]** In the above formula, the term "C<sub>1</sub> to C<sub>7</sub> alkyl" denotes such radicals as methyl, ethyl, n-propyl, isopropyl, n-butyl, iso-butyl, sec-butyl, tert-butyl, amyl, tert-amyl, hexyl and the like. The preferred "C<sub>1</sub> to C<sub>7</sub> alkyl" groups are methyl, iso-butyl, sec-butyl and iso-propyl.

**[0034]** The term "C<sub>1</sub> to C<sub>7</sub> substituted alkyl," denotes that the above C<sub>1</sub> to C<sub>7</sub> alkyl groups are substituted by one or more, and preferably one or two, halogen, hydroxy, protected hydroxy, oxo, protected oxo, C<sub>3</sub> to C<sub>7</sub> cycloalkyl, naphthyl, amino, protected amino, (monosubstituted)amino, protected (monosubstituted)amino, (disubstituted)amino, guanidino, protected guanidino, heterocyclic ring, substituted heterocyclic ring, imidazolyl, indolyl, pyrrolidinyl, C<sub>1</sub> to C<sub>7</sub> alkoxy, C<sub>1</sub> to C<sub>7</sub> acyl, C<sub>1</sub> to C<sub>7</sub> acyloxy, nitro, carboxy, protected carboxy, carbamoyl, carboxamide, protected carboxamide, N-(C<sub>1</sub> to C<sub>6</sub> alkyl)carboxamide, protected N-(C<sub>1</sub> to C<sub>6</sub> alkyl)carboxamide, N,N-di(C<sub>1</sub> to C<sub>6</sub> alkyl)carboxamide, cyano, methylsulfonylamino, thiol, C<sub>1</sub> to C<sub>4</sub> alkylthio or C<sub>1</sub> to C<sub>4</sub> alkylsulfonyl groups. The substituted alkyl groups may be substituted once or more, and preferably once or twice, with the same or with different substituents.

**[0035]** Examples of the above substituted alkyl groups include the 2-oxo-prop-1-yl, 3-oxo-but-1-yl, cyanomethyl, nitromethyl, chloromethyl, hydroxymethyl, tetrahydropyranyloxymethyl, trityloxymethyl, propionyloxymethyl, amino, methylamino, aminomethyl, dimethylamino, carboxymethyl,



allyloxycarbonylmethyl, allyloxycarbonylaminomethyl, methoxymethyl, ethoxymethyl, t-butoxymethyl, acetoxymethyl, chloromethyl, bromomethyl, iodomethyl, trifluoromethyl, 6-hydroxyhexyl, 2,4-dichloro(n-butyl), 2-aminopropyl, 1-chloroethyl, 2-chloroethyl, 1-bromoethyl, 2-chloroethyl, 1-fluoroethyl, 2-fluoroethyl, 1-iodoethyl, 2-iodoethyl, 1-chloropropyl, 2-chloropropyl, 3-chloropropyl, 1-bromopropyl, 2-bromopropyl, 3-bromopropyl, 1-fluoropropyl, 2-fluoropropyl, 3-fluoropropyl, 1-iodopropyl, 2-iodopropyl, 3-iodopropyl, 2-aminoethyl, 1-aminoethyl, N-benzoyl-2-aminoethyl, N-acetyl-2-aminoethyl, N-benzoyl-1-aminoethyl, N-acetyl-1-aminoethyl and the like.

**[0036]** The term "C<sub>1</sub> to C<sub>7</sub> alkoxy" as used herein denotes groups such as methoxy, ethoxy, n-propoxy, isopropoxy, n-butoxy, t-butoxy and like groups. A preferred alkoxy is methoxy. The term "C<sub>1</sub> to C<sub>7</sub> substituted alkoxy" means the alkyl portion of the alkoxy can be substituted in the same manner as in relation to C<sub>1</sub> to C<sub>7</sub> substituted alkyl. Similarly, the term "C<sub>1</sub> to C<sub>7</sub> phenylalkoxy" as used herein means "C<sub>1</sub> to C<sub>7</sub> alkoxy" bonded to a phenyl radical.

**[0037]** The substituent term "C<sub>3</sub> to C<sub>7</sub> cycloalkyl" includes the cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl or cycloheptyl rings. The substituent term "C<sub>3</sub> to C<sub>7</sub> substituted cycloalkyl" indicates the above cycloalkyl rings substituted by one or two halogen, hydroxy, protected hydroxy, C<sub>1</sub> to C<sub>4</sub> alkylthio, C<sub>1</sub> to C<sub>4</sub> alkylsulfoxide, C<sub>1</sub> to C<sub>4</sub> alkylsulfonyl, C<sub>1</sub> to C<sub>4</sub> substituted alkylthio, C<sub>1</sub> to C<sub>4</sub> substituted alkylsulfoxide, C<sub>1</sub> to C<sub>4</sub> substituted alkylsulfonyl, C<sub>1</sub> to C<sub>6</sub> alkyl, C<sub>1</sub> to C<sub>7</sub> alkoxy, C<sub>1</sub> to C<sub>6</sub> substituted alkyl, C<sub>1</sub> to C<sub>7</sub> alkoxy, oxo, protected oxo, (monosubstituted)amino, (disubstituted)amino, trifluoromethyl, carboxy, protected carboxy, phenyl, substituted phenyl, phenylthio, phenylsulfoxide, phenylsulfonyl, amino, or protected amino groups.

**[0038]** The term "substituted phenyl" specifies a phenyl group substituted with one or more, and preferably one or two, moieties chosen from the groups consisting of halogen, hydroxy, protected hydroxy, cyano, nitro, C<sub>1</sub> to C<sub>6</sub> alkyl, C<sub>1</sub> to C<sub>6</sub> substituted alkyl, C<sub>1</sub> to C<sub>7</sub> alkoxy, C<sub>1</sub> to C<sub>7</sub> substituted alkoxy, C<sub>1</sub> to C<sub>7</sub> acyl, C<sub>1</sub> to C<sub>7</sub> substituted acyl, C<sub>1</sub> to C<sub>7</sub> alkylthio, C<sub>1</sub> to C<sub>7</sub> acyloxy, carboxy, protected carboxy, carboxymethyl, protected carboxymethyl, hydroxymethyl, protected

hydroxymethyl, amino, protected amino, (monosubstituted)amino, protected (monosubstituted)amino, (disubstituted)amino, carboxamide, protected carboxamide, N-(C<sub>1</sub> to C<sub>6</sub> alkyl)carboxamide, protected N-(C<sub>1</sub> to C<sub>6</sub> alkyl)carboxamide, N, N-di(C<sub>1</sub> to C<sub>6</sub> alkyl)carboxamide, trifluoromethyl, N-((C<sub>1</sub> to C<sub>6</sub> alkyl)sulfonyl)amino, - (phenylsulfonyl)amino or phenyl, wherein the phenyl is substituted or unsubstituted, such that, for example, a biphenyl results.

**[0039]** Examples of the term "substituted phenyl" includes a mono- or di(halo)phenyl group such as 2, 3 or 4-chlorophenyl, 2,6-dichlorophenyl, 2,5-dichlorophenyl, 3,4-dichlorophenyl, 2, 3 or 4-bromophenyl, 3,4-dibromophenyl, 3-chloro-4-fluorophenyl, 2, 3 or 4-fluorophenyl and the like; a mono or di(hydroxy)phenyl group such as 2, 3 or 4-hydroxyphenyl, 2,4-dihydroxyphenyl, the protected-hydroxy derivatives thereof and the like; a nitrophenyl group such as 2, 3 or 4-nitrophenyl; a cyanophenyl group, for example, 2, 3 or 4-cyanophenyl; a mono- or di(alkyl)phenyl group such as 2, 3 or 4-methylphenyl, 2,4-dimethylphenyl, 2, 3 or 4-(iso-propyl)phenyl, 2, 3 or 4-ethylphenyl, 2, 3 or 4-(n-propyl)phenyl and the like; a mono or di(alkoxyl)phenyl group, for example, 2,6-dimethoxyphenyl, 2, 3 or 4-methoxyphenyl, 2, 3 or 4-ethoxyphenyl, 2, 3 or 4-(isopropoxy)phenyl, 2, 3 or 4-(t-butoxy)phenyl, 3-ethoxy-4-methoxyphenyl and the like; 2, 3 or 4-trifluoromethylphenyl; a mono- or dicarboxyphenyl or (protected carboxy)phenyl group such as 2, 3 or 4-carboxyphenyl or 2,4-di(protected carboxy)phenyl; a mono-or di(hydroxymethyl)phenyl or (protected hydroxymethyl)phenyl such as 2, 3, or 4-(protected hydroxymethyl)phenyl or 3,4-di(hydroxymethyl)phenyl; a mono- or di(aminomethyl)phenyl or (protected aminomethyl)phenyl such as 2, 3 or 4-(aminomethyl)phenyl or 2,4-(protected aminomethyl)phenyl; or a mono- or di(N-(methylsulfonylamino))phenyl such as 2, 3 or 4-(N-(methylsulfonylamino))phenyl. Also, the term "substituted phenyl" represents disubstituted phenyl groups wherein the substituents are different, for example, 3-methyl-4-hydroxyphenyl, 3-chloro-4-hydroxyphenyl, 2-methoxy-4-bromophenyl, 4-ethyl-2-hydroxyphenyl, 3-hydroxy-4-nitrophenyl, 2-hydroxy 4-chlorophenyl and the like.

**[0040]** The terms "halo" and "halogen" refer to the fluoro, chloro, bromo or

iodo atoms. There can be one or more halogen, which are the same or different. Preferred halogens are chloro and fluoro.

**[0041]** The term "substituted amino" refers to an amino group with one substituent chosen from the group consisting of phenyl, substituted phenyl, C<sub>1</sub> to C<sub>6</sub> alkyl, C<sub>1</sub> to C<sub>6</sub> substituted alkyl, C<sub>1</sub> to C<sub>7</sub> acyl, C<sub>1</sub> to C<sub>7</sub> substituted acyl, C<sub>2</sub> to C<sub>7</sub> alkenyl, C<sub>2</sub> to C<sub>7</sub> substituted alkenyl, C<sub>2</sub> to C<sub>7</sub> alkynyl, C<sub>2</sub> to C<sub>7</sub> substituted alkynyl, C<sub>7</sub> to C<sub>12</sub> phenylalkyl, C<sub>7</sub> to C<sub>12</sub> substituted phenylalkyl and heterocyclic ring. The substituted amino can additionally have an amino-protecting group as encompassed by the term "protected substituted amino."

**[0042]** The term "(disubstituted)amino" refers to an amino group with two substituents chosen from the group consisting of phenyl, substituted phenyl, C<sub>1</sub> to C<sub>6</sub> alkyl, C<sub>1</sub> to C<sub>6</sub> substituted alkyl, C<sub>1</sub> to C<sub>7</sub> acyl, C<sub>2</sub> to C<sub>7</sub> alkenyl, C<sub>2</sub> to C<sub>7</sub> alkynyl, C<sub>7</sub> to C<sub>12</sub> phenylalkyl, and C<sub>7</sub> to C<sub>12</sub> substituted phenylalkyl. The two substituents can be the same or different.

**[0043]** The term "C<sub>1</sub> to C<sub>4</sub> alkylthio" refers to sulfide groups such as methylthio, ethylthio, n-propylthio, isopropylthio, n-butylthio, t-butylthio and like groups.

**[0044]** The term "C<sub>1</sub> to C<sub>4</sub> substituted alkylthio," denotes that the C<sub>1</sub> to C<sub>4</sub> alkyl portion of this group may be substituted as described above in relation to "substituted alkyl."

**[0045]** The term "phenoxy" denotes a phenyl bonded to an oxygen atom, wherein the binding to the rest of the molecule is through the oxygen atom. The term "substituted phenoxy" specifies a phenoxy group substituted with one or more, and preferably one or two, moieties chosen from the groups consisting of halogen, hydroxy, protected hydroxy, cyano, nitro, C<sub>1</sub> to C<sub>12</sub> alkyl, C<sub>1</sub> to C<sub>12</sub> alkoxy, C<sub>1</sub> to C<sub>12</sub> substituted alkoxy, C<sub>1</sub> to C<sub>12</sub> acyl, C<sub>1</sub> to C<sub>12</sub> acyloxy, carboxy, protected carboxy, carboxymethyl, protected carboxymethyl, hydroxymethyl, protected hydroxymethyl, amino, protected amino, (monosubstituted)amino, protected (monosubstituted)amino, (disubstituted)amino, carboxamide, protected carboxamide, N-(C<sub>1</sub> to C<sub>12</sub> alkyl)carboxamide, protected N-(C<sub>1</sub> to C<sub>12</sub> alkyl)carboxamide, N, N-di(C<sub>1</sub> to C<sub>12</sub> alkyl)carboxamide, trifluoromethyl, N-((C<sub>1</sub> to

C<sub>12</sub> alkyl)sulfonyl)amino and N- (phenylsulfonyl)amino.

**[0046]** The terms "C<sub>7</sub> to C<sub>18</sub> substituted phenylalkyl" and "C<sub>1</sub> to C<sub>12</sub> substituted heterocycloalkyl" denote a C<sub>7</sub> to C<sub>18</sub> phenylalkyl group or C<sub>1</sub> to C<sub>12</sub> heterocycloalkyl substituted (on the alkyl or, where applicable, phenyl or heterocyclic portion) with one or more, and preferably one or two, groups chosen from halogen, hydroxy, protected hydroxy, oxo, protected oxo, amino, protected amino, substituted amino, protected substituted amino, (disubstituted)amino, guanidino, protected guanidino, heterocyclic ring, substituted heterocyclic ring, C<sub>1</sub> to C<sub>12</sub> alkyl, C<sub>1</sub> to C<sub>12</sub> substituted alkyl, C<sub>1</sub> to C<sub>12</sub> alkoxy, C<sub>1</sub> to C<sub>12</sub> substituted alkoxy, C<sub>1</sub> to C<sub>12</sub> acyl, C<sub>1</sub> to C<sub>12</sub> substituted acyl, C<sub>1</sub> to C<sub>12</sub> acyloxy, nitro, carboxy, protected carboxy, carbamoyl, carboxamide, protected carboxamide, N-(C<sub>1</sub> to C<sub>12</sub> alkyl)carboxamide, protected N-(C<sub>1</sub> to C<sub>12</sub> alkyl)carboxamide, N, N-(C<sub>1</sub> to C<sub>12</sub> dialkyl)carboxamide, cyano, N-(C<sub>1</sub> to C<sub>12</sub> alkylsulfonyl)amino, thiol, C<sub>1</sub> to C<sub>10</sub> alkylthio, C<sub>1</sub> to C<sub>10</sub> alkylsulfonyl groups; and/or the phenyl group may be substituted with one or more, and preferably one or two, substituents chosen from halogen, hydroxy, protected hydroxy, cyano, nitro, C<sub>1</sub> to C<sub>12</sub> alkyl, C<sub>1</sub> to C<sub>12</sub> substituted alkyl, C<sub>1</sub> to C<sub>12</sub> alkoxy, C<sub>1</sub> to C<sub>12</sub> substituted alkoxy, C<sub>1</sub> to C<sub>12</sub> acyl, C<sub>1</sub> to C<sub>12</sub> substituted acyl, C<sub>1</sub> to C<sub>12</sub> acyloxy, carboxy, protected carboxy, carboxymethyl, protected carboxymethyl, hydroxymethyl, protected hydroxymethyl, amino, protected amino, (monosubstituted)amino, protected (monosubstituted)amino, (disubstituted)amino, carboxamide, protected carboxamide, N-(C<sub>1</sub> to C<sub>12</sub> alkyl)carboxamide, protected N-(C<sub>1</sub> to C<sub>12</sub> alkyl)carboxamide, N, N-di(C<sub>1</sub> to C<sub>12</sub> alkyl)carboxamide, trifluoromethyl, N-((C<sub>1</sub> to C<sub>12</sub> alkyl)sulfonyl)amino, N-(phenylsulfonyl)amino, cyclic C<sub>2</sub> to C<sub>12</sub> alkylene or a phenyl group, substituted or unsubstituted, for a resulting biphenyl group. The substituted alkyl, phenyl or heterocyclic groups may be substituted with one or more, and preferably one or two, substituents which can be the same or different.

**[0047]** Examples of the term "C<sub>7</sub> to C<sub>18</sub> substituted phenylalkyl" include groups such as 2-phenyl-1-chloroethyl, 2-(4-methoxyphenyl)ethyl, 4-(2,6-dihydroxy phenyl)n-hexyl, 2-(5-cyano-3-methoxyphenyl)n-pentyl, 3-(2,6-dimethylphenyl)n-propyl, 4-chloro-3-aminobenzyl, 6-(4-methoxyphenyl)-3-carboxy(n-hexyl), 5-(4-

aminomethylphenyl)- 3-(aminomethyl)n-pentyl, 5-phenyl-3-oxo-n-pent-1-yl and the like.

**[0048]** The term "C<sub>7</sub> to C<sub>18</sub> phenylalkylene" specifies a C<sub>7</sub> to C<sub>18</sub> phenylalkyl, as defined above, where the phenylalkyl radical is bonded at two different positions connecting together two separate additional groups. The definition includes groups of the formula: -phenyl-alkyl-, -alkyl-phenyl- and -alkyl-phenyl-alkyl-. Substitutions on the phenyl ring can be 1,2, 1,3 or 1,4.

**[0049]** C<sub>7</sub> to C<sub>18</sub> phenylalkylenes include, for example, 1,4-tolylene and 1,3-xylylene.

**[0050]** The terms "cyclic C<sub>2</sub> to C<sub>7</sub> alkylene," "substituted cyclic C<sub>2</sub> to C<sub>7</sub> alkylene," "cyclic C<sub>2</sub> to C<sub>7</sub> heteroalkylene," and "substituted cyclic C<sub>2</sub> to C<sub>7</sub> heteroalkylene," defines such a cyclic group bonded ("fused") to the phenyl radical resulting in a bicyclic ring system. The cyclic group may be saturated or contain one or two double bonds. Furthermore, the cyclic group may have one or two methylene or methine groups replaced by one or two oxygen, nitrogen or sulfur atoms which are the cyclic C<sub>2</sub> to C<sub>7</sub> heteroalkylene.

**[0051]** The cyclic alkylene or heteroalkylene group may be substituted once or twice by the same or different substituents which, if appropriate, can be connected to another part of the compound (e.g., alkylene) selected from the group consisting of the following moieties: hydroxy, protected hydroxy, carboxy, protected carboxy, oxo, protected oxo, C<sub>1</sub> to C<sub>4</sub> acyloxy, formyl, C<sub>1</sub> to C<sub>12</sub> acyl, C<sub>1</sub> to C<sub>12</sub> alkyl, C<sub>1</sub> to C<sub>7</sub> alkoxy, C<sub>1</sub> to C<sub>10</sub> alkylthio, C<sub>1</sub> to C<sub>10</sub> alkylsulfoxide, C<sub>1</sub> to C<sub>10</sub> alkylsulfonyl, halo, amino, protected amino, substituted amino, protected substituted amino, (disubstituted)amino, hydroxymethyl or a protected hydroxymethyl.

**[0052]** The cyclic alkylene or heteroalkylene group fused onto the benzene radical can contain two to ten ring members, but it preferably contains three to six members. Examples of such saturated cyclic groups are when the resultant bicyclic ring system is 2,3-dihydro-indanyl and a tetralin ring. When the cyclic groups are unsaturated, examples occur when the resultant bicyclic ring system is a naphthyl ring or indolyl. Examples of fused cyclic groups which each contain

one nitrogen atom and one or more double bond, preferably one or two double bonds, are when the benzene radical is fused to a pyridino, pyrano, pyrrolo, pyridinyl, dihydropyrrolo, or dihydropyridinyl ring. Examples of fused cyclic groups which each contain one oxygen atom and one or two double bonds are when the benzene radical ring is fused to a furo, pyrano, dihydrofurano, or dihydropyrano ring. Examples of fused cyclic groups which each have one sulfur atom and contain one or two double bonds are when the benzene radical is fused to a thieno, thiopyrano, dihydrothieno or dihydrothiopyrano ring. Examples of cyclic groups which contain two heteroatoms selected from sulfur and nitrogen and one or two double bonds are when the benzene radical ring is fused to a thiazolo, isothiazolo, dihydrothiazolo or dihydroisothiazolo ring. Examples of cyclic groups which contain two heteroatoms selected from oxygen and nitrogen and one or two double bonds are when the benzene ring is fused to an oxazolo, isoxazolo, dihydrooxazolo or dihydroisoxazolo ring. Examples of cyclic groups which contain two nitrogen heteroatoms and one or two double bonds occur when the benzene ring is fused to a pyrazolo, imidazolo, dihydropyrazolo or dihydroimidazolo ring or pyrazinyl.

**[0053]** The term "heterocycle" or "heterocyclic ring" denotes optionally substituted five-membered to eight-membered rings that have 1 to 4 heteroatoms, such as oxygen, sulfur and/or nitrogen, in particular nitrogen, either alone or in conjunction with sulfur or oxygen ring atoms. These five-membered to eight-membered rings may be saturated, fully unsaturated or partially unsaturated, with fully saturated rings being preferred. Preferred heterocyclic rings include morpholino, piperidinyl, piperazinyl, 2-amino-imidazolyl, tetrahydrofurano, pyrrolo, tetrahydrothiophen-yl, hexylmethyleneimino and heptylmethyleneimino.

**[0054]** The term "substituted heterocycle" or "substituted heterocyclic ring" means the above-described heterocyclic ring is substituted with, for example, one or more, and preferably one or two, substituents which are the same or different which substituents can be halogen, hydroxy, protected hydroxy, cyano, nitro, C<sub>1</sub> to C<sub>12</sub> alkyl, C<sub>1</sub> to C<sub>12</sub> alkoxy, C<sub>1</sub> to C<sub>12</sub> substituted alkoxy, C<sub>1</sub> to C<sub>12</sub> acyl,

C<sub>1</sub> to C<sub>12</sub> acyloxy, carboxy, protected carboxy, carboxymethyl, protected carboxymethyl, hydroxymethyl, protected hydroxymethyl, amino, protected amino, substituted amino, protected substituted amino, (disubstituted)amino carboxamide, protected carboxamide, N-(C<sub>1</sub> to C<sub>12</sub> alkyl)carboxamide, protected N-(C<sub>1</sub> to C<sub>12</sub> alkyl)carboxamide, N, N-di(C<sub>1</sub> to C<sub>12</sub> alkyl)carboxamide, trifluoromethyl, N-((C<sub>1</sub> to C<sub>12</sub> alkyl)sulfonyl)amino, N-(phenylsulfonyl)amino, heterocycle or substituted heterocycle groups.

**[0055]** One or more of the compounds of the invention, even within a given library, may be present as a salt. The term "salt" encompasses those salts that form with the carboxylate anions and amine nitrogens and include salts formed with the organic and inorganic anions and cations discussed below. Furthermore, the term includes salts that form by standard acid-base reactions with basic groups (such as amino groups) and organic or inorganic acids. Such acids include hydrochloric, sulfuric, phosphoric, acetic, succinic, citric, lactic, maleic, fumaric, palmitic, cholic, pamoic, mucic, D-glutamic, D-camphoric, glutaric, phthalic, tartaric, lauric, stearic, salicylic, methanesulfonic, benzenesulfonic, sorbic, picric, benzoic, cinnamic, and like acids.

**[0056]** The term "organic or inorganic cation" refers to counter-ions for the carboxylate anion of a carboxylate salt. The counter-ions are chosen from the alkali and alkaline earth metals, (such as lithium, sodium, potassium, barium, aluminum and calcium); ammonium and mono-, di- and tri-alkyl amines such as trimethylamine, cyclohexylamine; and the organic cations, such as dibenzylammonium, benzylammonium, 2-hydroxyethylammonium, bis(2-hydroxyethyl)ammonium, phenylethylbenzylammonium, dibenzylethylenediammonium, and like cations. See, for example, "Pharmaceutical Salts," Berge et al., J. Pharm. Sci., 66:1-19 (1977). Other cations encompassed by the above term include the protonated form of procaine, quinine and N-methylglucosamine, and the protonated forms of basic amino acids such as glycine, ornithine, histidine, phenylglycine, lysine and arginine. Furthermore, any zwitterionic form of the instant compounds formed by a carboxylic acid and an amino group is referred to by this term. For example, a

cation for a carboxylate anion will exist when R<sub>2</sub> or R<sub>3</sub> is substituted with a (quaternary ammonium)methyl group. A preferred cation for the carboxylate anion is the sodium cation.

**[0057]** The compounds of the invention can also exist as solvates and hydrates. Thus, these compounds may crystallize with, for example, waters of hydration, or one, a number of, or any fraction thereof of molecules of the mother liquor solvent. The solvates and hydrates of such compounds are included within the scope of this invention.

**[0058]** One or more compounds of the invention, even when in a library, can be in the biologically active ester form, such as the non-toxic, metabolically-labile ester-form. Such ester forms induce increased blood levels and prolong the efficacy of the corresponding non-esterified forms of the compounds. Ester groups which can be used include the lower alkoxymethyl groups, for example, methoxymethyl, ethoxymethyl, isopropoxymethyl and the like; the -(C<sub>1</sub> to C<sub>7</sub>) alkoxyethyl groups, for example methoxyethyl, ethoxyethyl, propoxyethyl, isopropoxyethyl and the like; the 2-oxo-1,3-dioxolen-4-ylmethyl groups, such as 5-methyl-2-oxo-1,3-dioxolen-4-ylmethyl, 5-phenyl-2-oxo-1,3-dioxolen-4-ylmethyl and the like; the C<sub>1</sub> to C<sub>4</sub> alkylthiomethyl groups, for example methylthiomethyl, ethylthiomethyl, iso-propylthiomethyl and the like; the acyloxymethyl groups, for example pivaloyloxymethyl, pivaloyloxyethyl, -acetoxymethyl and the like; the ethoxycarbonyl-1-methyl group; the -acetoxoethyl; the 1-(C<sub>1</sub> to C<sub>7</sub> alkyloxycarbonyloxy)ethyl groups such as the 1-(ethoxycarbonyloxy)ethyl group; and the 1-(C<sub>1</sub> to C<sub>7</sub> alkylaminocarbonyloxy)ethyl groups such as the 1-(methylaminocarbonyloxy)ethyl group.

**[0059]** The term "amino acid" includes any one of the twenty naturally-occurring amino acids or the D-form of any one of the naturally-occurring amino acids. In addition, the term "amino acid" also includes other non-naturally occurring amino acids besides the D-amino acids, which are functional equivalents of the naturally-occurring amino acids. Such non-naturally-occurring amino acids include, for example, norleucine ("Nle"), norvaline ("Nva"), L- or D-naphthalanine, ornithine ("Orn"), homoarginine (homoArg) and others well known



in the peptide art, such as those described in M. Bodanzsky, "Principles of Peptide Synthesis," 1st and 2nd revised ed., Springer-Verlag, New York, NY, 1984 and 1993, and Stewart and Young, "Solid Phase Peptide Synthesis," 2nd ed., Pierce Chemical Co., Rockford, IL, 1984. Amino acids and amino acid analogs can be purchased commercially (Sigma Chemical Co.; Advanced Chemtech) or synthesized using methods known in the art.

**[0060]** The term "functionalized resin" means any resin, crosslinked or otherwise, where functional groups have been introduced into the resin, as is common in the art. Such resins include, for example, those functionalized with amino, alkylhalo, formyl or hydroxy groups. Such resins which can serve as solid supports are well known in the art and include, for example, 4-methylbenzhydrylamine-copoly(styrene-1% divinylbenzene) (MBHA), 4-hydroxymethylphenoxymethyl-copoly(styrene-1% divinylbenzene), 4-oxymethyl-phenyl-acetamido-copoly(styrene-1% divinylbenzene)(Wang), 4-(oxymethyl)-phenylacetamido methyl (Pam), and Tentagel™, from Rapp Polymere GmbH, trialkoxy-diphenyl-methyl ester- copoly(styrene-1% divinylbenzene)(RINK) all of which are commercially available. Other functionalized resins are known in the art and can be used without departure from the scope of the current invention. Such resins may include those described in Jung, G., Combinatorial Peptide and Nonpeptide Libraries, A Handbook (VCH Verlag, 1996) or Bunin, B. A., The Combinatorial Index (Academic Press, 1998).

**[0061]** As used herein, a "combinatorial library" is an intentionally created collection of differing molecules which can be prepared by the means provided below or otherwise and screened for biological activity in a variety of formats (e.g., libraries of soluble molecules, libraries of compounds attached to resin beads, silica chips or other solid supports). A "combinatorial library," as defined above, involves successive rounds of chemical syntheses based on a common starting structure. The combinatorial libraries can be screened in any variety of assays, such as those detailed below as well as others useful for assessing their biological activity. The combinatorial libraries will generally have at least one active compound and are generally prepared such that the compounds are in

equimolar quantities.

**[0062]** A combinatorial library of the invention can contain one or more of the above-described compounds. The invention further provides a combinatorial library containing five or more of the above-described compounds. In another embodiment of the invention, a combinatorial library can contain ten or more of the above-described compounds. In yet another embodiment of the invention, a combinatorial library can contain fifty or more of the above-described compounds. If desired, a combinatorial library of the invention can contain 100,000 or more, or even 1,000,000 or more, of the above-described compounds.

**[0063]** By way of example, the preparation of the combinatorial libraries can use the "split resin approach." The split resin approach is described by, for example, U.S. Patent 5,010,175 to Rutter, WO PCT 91/19735 to Simon, and Gallop et al., *J. Med. Chem.*, 37:1233-1251 (1994).

**[0064]** For preparing pharmaceutical compositions containing compounds of the invention, inert, pharmaceutically acceptable carriers are used. The pharmaceutical carrier can be either solid or liquid. Solid form preparations include, for example, powders, tablets, dispersible granules, capsules, cachets, and suppositories.

**[0065]** A solid carrier can be one or more substances which can also act as diluents, flavoring agents, solubilizers, lubricants, suspending agents, binders, or tablet disintegrating agents; it can also be an encapsulating material.

**[0066]** In powders, the carrier is generally a finely divided solid which is in a mixture with the finely divided active component. In tablets, the active compound is mixed with the carrier having the necessary binding properties in suitable proportions and compacted in the shape and size desired.

**[0067]** For preparing pharmaceutical composition in the form of suppositories, a low-melting wax such as a mixture of fatty acid glycerides and cocoa butter is first melted and the active ingredient is dispersed therein by, for example, stirring. The molten homogeneous mixture is then poured into convenient-sized molds and allowed to cool and solidify.

**[0068]** Powders and tablets preferably contain between about 5% to about 70% by weight of the active ingredient. Suitable carriers include, for example, magnesium carbonate, magnesium stearate, talc, lactose, sugar, pectin, dextrin, starch, tragacanth, methyl cellulose, sodium carboxymethyl cellulose, a low-melting wax, cocoa butter and the like.

**[0069]** The pharmaceutical compositions can include the formulation of the active compound with encapsulating material as a carrier providing a capsule in which the active component (with or without other carriers) is surrounded by a carrier, which is thus in association with it. In a similar manner, cachets are also included. Tablets, powders, cachets, and capsules can be used as solid dosage forms suitable for oral administration.

**[0070]** Liquid pharmaceutical compositions include, for example, solutions suitable for oral or parenteral administration, or suspensions, and emulsions suitable for oral administration. Sterile water solutions of the active component or sterile solutions of the active component in solvents comprising water, ethanol, or propylene glycol are examples of liquid compositions suitable for parenteral administration.

**[0071]** Sterile solutions can be prepared by dissolving the active component in the desired solvent system, and then passing the resulting solution through a membrane filter to sterilize it or, alternatively, by dissolving the sterile compound in a previously sterilized solvent under sterile conditions.

**[0072]** Aqueous solutions for oral administration can be prepared by dissolving the active compound in water and adding suitable flavorants, coloring agents, stabilizers, and thickening agents as desired. Aqueous suspensions for oral use can be made by dispersing the finely divided active component in water together with a viscous material such as natural or synthetic gums, resins, methyl cellulose, sodium carboxymethyl cellulose, and other suspending agents known to the pharmaceutical formulation art.

**[0073]** Preferably, the pharmaceutical composition is in unit dosage form. In such form, the composition is divided into unit doses containing appropriate quantities of the active piperidine-3-carboxamide. The unit dosage form can be a

packaged preparation, the package containing discrete quantities of the preparation, for example, packeted tablets, capsules, and powders in vials or ampules. The unit dosage form can also be a capsule, cachet, or tablet itself, or it can be the appropriate number of any of these packaged forms.

**[0074]** As pharmaceutical compositions for treating infections, pain, or any other indication the compounds of the present invention are generally in a pharmaceutical composition so as to be administered to a subject at dosage levels of from 0.7 to 7000 mg per day, and preferably 1 to 500 mg per day, for a normal human adult of approximately 70 kg of body weight, this translates into a dosage of from 0.01 to 100 mg/kg of body weight per day. The specific dosages employed, however, can be varied depending upon the requirements of the patient, the severity of the condition being treated, and the activity of the compound being employed. The determination of optimum dosages for a particular situation is within the skill of the art.

**[0075]** Variant piperidine-3-carboxamide derivative compounds and combinatorial libraries can be prepared as shown in figures 1 and 2 in order to achieve a high level of diversity.

**[0076]** Resins suitable for use in the present invention can easily be determined by one skilled in the art. Such resins include but are not limited to polystyrene resin (e.g. Wang resin : *p*-benzyloxybenzyl alcohol-polystyrene) and PEG-grafted polystyrene resin (e.g. Tentagel, Argogel).

**[0077]** Other suitable resins known in the art can be found in "Solid Phase Synthesis and Combinatorial Technologies", Seneci, P.; John Wiley and Sons, 2000, p 1-45.

**[0078]** The resulting compound can be cleaved from the resin. Resin-bound piperidine-3-carboxamide derivative compounds can be cleaved by treating them, for example, with HF. They can also be cleaved with TFA/DCM, provided that TFA sensitive protecting group such as Boc are not used in the synthetic scheme. The compounds can be extracted from the spent resin, for example, with AcOH.

**[0079]** The nonsupport-bound combinatorial libraries can be screened as

single compounds. In addition, the nonsupport-bound combinatorial libraries can be screened as mixtures in solution in assays such as radio-receptor inhibition assays, anti-bacterial assays, anti-fungal assays, calmodulin-dependent phosphodiesterase (CaMPDE) assays and phosphodiesterase (PDE) assays, as described in detail below. Deconvolution of highly active mixtures can then be carried out by iterative or positional scanning methods. These techniques, the iterative approach or the positional scanning approach, can be utilized for finding other active compounds within the combinatorial libraries of the present invention using any one of the below-described assays or others well known in the art.

**[0080]** The iterative approach is well-known and is set forth in general in Houghten *et al.*, *Nature*, 354, 84-86 (1991) and Dooley *et al.*, *Science*, 266, 2019-2022 (1994), both of which are incorporated herein by reference. In the iterative approach, for example, sub-libraries of a molecule having three variable groups are made wherein the first variable is defined. Each of the compounds with the defined variable group is reacted with all of the other possibilities at the other two variable groups. These sub-libraries are each tested to define the identity of the second variable in the sub-library having the highest activity in the screen of choice. A new sub-library with the first two variable positions defined is reacted again with all the other possibilities at the remaining undefined variable position. As before, the identity of the third variable position in the sub-library having the highest activity is determined. If more variables exist, this process is repeated for all variables, yielding the compound with each variable contributing to the highest desired activity in the screening process. Promising compounds from this process can then be synthesized on larger scale in traditional single-compound synthetic methods for further biological investigation.

**[0081]** The positional-scanning approach has been described for various combinatorial libraries as described, for example, in R. Houghten *et al.* PCT/US91/08694 and U.S. Patent 5,556,762, both of which are incorporated herein by reference. In the positional scanning approach, sublibraries are made defining only one variable with each set of sublibraries and all possible sublibraries with each single variable defined (and all other possibilities at all of

**[0082]** Individual compounds and pharmaceutical compositions containing the compounds, as well as methods of using the same, are included within the scope of the present invention. The compounds of the present invention can be used for a variety of purposes and indications and as medicaments for any such purposes and indications. For example, piperidine-3-carboxamide derivative compounds of the present invention can be used as pesticides, acaricides, receptor agonists or antagonists and antimicrobial agents, including antibacterial or antiviral agents. The libraries can be screened in any variety of melanocortin receptor and related activity assays, such as those detailed below as well as others known in the art. Additionally, the subject compounds can be useful as analgesics. Assays which can be used to test the biological activity of the instant compounds include antimicrobial assays, a competitive enzyme-linked immunoabsorbent assay and radio-receptor assays, as described below.

**[0083]** The melanocortin (MC) receptors are a group of cell surface proteins that mediate a variety of physiological effects, including regulation of adrenal gland function such as production of the glucocorticoids cortisol and aldosterone; control of melanocyte growth and pigment production; thermoregulation; immunomodulation; and analgesia. Five distinct MC receptors have been cloned and are expressed in a variety of tissues, including melanocytes, adrenal cortex, brain, gut, placenta, skeletal muscle, lung, spleen, thymus, bone marrow, pituitary, gonads and adipose tissue (Tatro, Neuroimmunomodulation 3:259-284 (1996)). Three MC receptors, MCR-1, MCR-3 and MCR-4, are expressed in

brain tissue (Xia et al., Neuroreport 6:2193-2196 (1995)).

**[0084]** A variety of ligands termed melanocortins function as agonists that stimulate the activity of MC receptors. The melanocortins include melanocyte-stimulating hormones (MSH) such as  $\alpha$ -MSH,  $\beta$ -MSH and  $\gamma$ -MSH, as well as adrenocorticotrophic hormone (ACTH). Individual ligands can bind to multiple MC receptors with differing relative affinities. The variety of ligands and MC receptors with differential tissue-specific expression likely provides the molecular basis for the diverse physiological effects of melanocortins and MC receptors. For example,  $\alpha$ -MSH antagonizes the actions of immunological substances such as cytokines and acts to modulate fever, inflammation and immune responses (Catania and Lipton, Annals N. Y. Acad. Sci. 680:412-423 (1993)).

**[0085]** The role of certain specific MC receptors in some of the physiological effects described above for MC receptors has been elucidated. For example, MCR-1 is involved in pain and inflammation. MCR-1 mRNA is expressed in neutrophils (Catania et al., Peptides 17:675-679 (1996)). The anti-inflammatory agent  $\alpha$ -MSH was found to inhibit migration of neutrophils. Thus, the presence of MCR-1 in neutrophils correlates with the anti-inflammatory activity of  $\alpha$ -MSH.

**[0086]** An interesting link of MC receptors to regulation of food intake and obesity has recently been described. The brain MC receptor MCR-4 has been shown to function in the regulation of body weight and food intake. Mice in which MCR-4 has been knocked out exhibit weight gain (Huszar et al., Cell 88:131-141 (1997)). In addition, injection into brain of synthetic peptides that mimic melanocortins and bind to MCR-4 caused suppressed feeding in normal and mutant obese mice (Fan et al., Nature 385:165-168 (1997)). These results indicate that the brain MC receptor MCR-4 functions in regulating food intake and body weight.

**[0087]** Due to the varied physiological activities of MC receptors, high affinity ligands of MC receptors could be used to exploit the varied physiological responses of MC receptors by functioning as potential therapeutic agents or as lead compounds for the development of therapeutic agents. Furthermore, due to

the effect of MC receptors on the activity of various cytokines, high affinity MC receptor ligands could also be used to regulate cytokine activity.

**[0088]** A variety of assays can be used to identify or characterize MC receptor ligands of the invention. For example, the ability of a piperidine-3-carboxamide derivative compound to compete for binding of a known MC receptor ligand can be used to assess the affinity and specificity of a piperidine-3-carboxamide derivative compound for one or more MC receptors. Any MC receptor ligand can be used so long as the ligand can be labeled with a detectable moiety. The detectable moiety can be, for example, a radiolabel, fluorescent label or chromophore, or any detectable functional moiety so long as the MC receptor ligand exhibits specific MC receptor binding. A particularly useful detectable MC receptor ligand for identifying and characterizing other MC receptor ligands is 125I-HP 467, which has the amino acid sequence Ac-Nle-Gln-His-(p(I)-D-Phe)-Arg-(D-Trp)-Gly-NH<sub>2</sub> and is described in Dooley et al., "Melanocortin Receptor Ligands and Methods of Using Same," U.S. patent application 09/027,108, filed February 20, 1998, which is incorporated herein by reference. HP 467 is a *para*-iodinated form of HP 228.

**[0089]** Using assay methods such as those described above, binding kinetics and competition with radiolabeled HP 467 can confirm that piperidine-3-carboxamide derivative compounds of the invention bind to one or more MC receptors. Furthermore, piperidine-3-carboxamide derivative compounds of the invention can exhibit a range of affinities and specificity for various MC receptors.

**[0090]** The invention provides MC receptor ligands that can bind to several MC receptors with similar affinity. In addition, the invention also provides MC receptor ligands that can be selective for one or more MC receptors. As used herein, the term "selective" means that the affinity of a MC receptor ligand differs between one MC receptor and another by about 10-fold, generally about 20- to 50-fold, and particularly about 100-fold. In some cases, a MC receptor ligand having broad specificity is desired. In other cases, it is desirable to use MC receptor ligands having selectivity for a particular MC receptor. For example, MCR-1 ligands are particularly useful for treating pain and inflammation, whereas



MCR-4 ligands are useful for treating obesity. The binding characteristics and specificity of a given MC receptor ligand can be selected based on the particular disease or physiological effect that is desired to be altered.

**[0091]** Another assay useful for identifying or characterizing MC receptor ligands measures signaling of MC receptors. MC receptors are G protein-coupled receptors that couple to adenylate cyclase and produce cAMP. Therefore, measuring cAMP production in a cell expressing a MC receptor and treated with a MC receptor ligand can be used to assess the function of the MC receptor ligand in activating a MC receptor.

**[0092]** Ligands for MC-3 that can alter the activity of an MC-3 receptor can be useful for treating sexual dysfunction and other conditions or conditions associated with MC-3 such as inflammation. Other MC-3-associated conditions that can be treated with the MC-3 receptor ligands include disuse deconditioning; organ damage such as organ transplantation or ischemic injury; adverse reactions associated with cancer chemotherapy; diseases such as atherosclerosis that are mediated by free radicals and nitric oxide action; bacterial endotoxic sepsis and related shock; adult respiratory distress syndrome; and autoimmune or other patho-immunogenic diseases or reactions such as allergic reactions or anaphylaxis, rheumatoid arthritis, inflammatory bowel disease, ulcerative colitis, glomerulonephritis, systemic lupus erythematosus, transplant atherosclerosis and parasitic mediated immune dysfunctions such as Chagas's disease.

**[0093]** The invention further provides a method for treating an MC-3-associated condition in a subject. The term "MC-3-associated condition" includes any condition or condition mediated by MC-3 or can be affected by binding an MC-3 ligand. Such conditions include inflammation and sexual dysfunction.

**[0094]** The term "sexual dysfunction" herein means any condition that inhibits or impairs normal sexual function, including coitus. However, the term need not be limited to physiological conditions, but may include psychogenic conditions or perceived impairment without a formal diagnosis of pathology.

**[0095]** In males, sexual dysfunction includes erectile dysfunction. The term "erectile dysfunction" or "impotence" means herein the inability or impaired ability to attain or sustain an erection that would be of satisfactory rigidity for coitus. Sexual dysfunction in males can also include premature ejaculation and priapism, which is a condition of prolonged and sometimes painful erection unrelated to sexual activity, often associated with sickle-cell disease.

**[0096]** In females, sexual dysfunction includes sexual arousal disorder. The term "sexual arousal disorder" means herein a persistent or recurrent failure to attain or maintain the lubrication-swelling response of sexual excitement until completion of sexual activity. Sexual dysfunction in females can also include inhibited orgasm and dyspareunia, which is painful or difficult coitus. Sexual dysfunction can also be manifested as inhibited sexual desire or inhibited lordosis behavior in animals.

**[0097]** In addition, the ability of the compounds to inhibit bacterial growth, and therefore be useful to that infection, can be determined by methods well known in the art. Compounds of the present invention can be shown to have antimicrobial activity by the *in vitro* antimicrobial activity assay described below and, therefore, are useful as antimicrobial agents.

**[0098]** Moreover, an exemplary *in vitro* antimicrobial activity assay is described in Blondelle and Houghten, *Biochemistry* 30:4671-4678 (1991), which is incorporated herein by reference. In brief, *Staphylococcus aureus* ATCC 29213 (Rockville, MD) is grown overnight at 37°C in Mueller-Hinton broth, then re-inoculated and incubated at 37°C to reach the exponential phase of bacterial growth (i.e., a final bacterial suspension containing 10<sup>5</sup> to 5 x 10<sup>5</sup> colony-forming units/ml). The concentration of cells is established by plating 100 µl of the culture solution using serial dilutions (e.g., 10<sup>-2</sup>, 10<sup>-3</sup> and 10<sup>-4</sup>) onto solid agar plates. In 96-well tissue culture plates, compounds, individual or in mixtures, are added to the bacterial suspension at concentrations derived from serial two-fold dilutions ranging from 1500 to 2.9 µg/ml. The plates are incubated overnight at 37°C and the growth determined at each concentration by OD<sub>620</sub> nm. The IC<sub>50</sub>

(the concentration necessary to inhibit 50% of the growth of the bacteria) can then be calculated.

**[0099]** The competitive ELISA method which can be used here is a modification of the direct ELISA technique described previously in Appel et al., J. Immunol. 144:976-983 (1990), which is incorporated herein by reference. It differs only in the MAb addition step. Briefly, multi-well microplates are coated with the antigenic peptide (Ac-GASPYPNLSNQQT-NH<sub>2</sub>) at a concentration of 100 pmol/50  $\mu$ l. After blocking, 25  $\mu$ l of a 1.0 mg/ml solution of each mixture of a synthetic combinatorial library (or individual compound) is added, followed by MAb 125-10F3 (Appel et al., *supra*) (25  $\mu$ l per well). The MAb is added at a fixed dilution in which the bicyclic guanidine in solution effectively competes for MAb binding with the antigenic peptide adsorbed to the plate. The remaining steps are the same as for direct ELISA. The concentration of compound necessary to inhibit 50% of the MAb binding to the control peptide on the plate (IC<sub>50</sub>) is determined by serial dilutions of the compound.

**[0100]** Alternative screening can be done with radio-receptor assays. The radio-receptor assay, can be selective for any one of the  $\mu$ ,  $\kappa$ , or  $\delta$  opiate receptors. Compounds of the present invention can be useful *in vitro* for the diagnosis of relevant opioid receptor subtypes, such as  $\kappa$ , in the brain and other tissue samples. Similarly, the compounds can be used *in vivo* diagnostically to localize opioid receptor subtypes.

**[0101]** The radio-receptor assays are also an indication of the compounds' analgesic properties as described, for example, in Dooley et al., *Proc. Natl. Acad. Sci.*, 90:10811-10815 (1993). For example, it can be envisioned that these compounds can be used for therapeutic purposes to block the peripheral effects of a centrally acting pain killer. For instance, morphine is a centrally acting pain killer. Morphine, however, has a number of deleterious effects in the periphery which are not required for the desired analgesic effects, such as constipation and pruritus (itching). While it is known that the many compounds do not readily cross the blood-brain barrier and, therefore, elicit no central effect, the subject

compounds can have value in blocking the periphery effects of morphine, such as constipation and pruritus. Accordingly, the subject compounds can also be useful as drugs, namely as analgesics, or to treat pathologies associated with other compounds which interact with the opioid receptor system.

**[0102]** Additionally, such compounds can be tested in a  $\sigma$  receptor assay. Ligands for the  $\sigma$  receptor can be useful as antipsychotic agents, as described in Abou-Gharbia et al., *Annual Reports in Medicinal Chemistry*, 28:1-10 (1993).

**[0103]** Radio-receptor assays can be performed with particulate membranes prepared using a modification of the method described in Pasternak et al., *Mol. Pharmacol.* 11:340-351 (1975), which is incorporated herein by reference. Rat brains frozen in liquid nitrogen can be obtained from Rockland (Gilbertsville, PA). The brains are thawed, the cerebella removed and the remaining tissue weighed. Each brain is individually homogenized in 40 ml Tris-HCl buffer (50 mM, pH 7.4, 4°C) and centrifuged (Sorvall® RC5C SA-600: Du Pont, Wilmington, DE) (16,000 rpm) for 10 minutes. The pellets are resuspended in fresh Tris-HCl buffer and incubated at 37°C for 40 minutes. Following incubation, the suspensions are centrifuged as before, the resulting pellets resuspended in 100 volumes of Tris buffer and the suspensions combined. Membrane suspensions are prepared and used in the same day. Protein content of the crude homogenates generally range from 0.15-0.2 mg/ml as determined using the method described in Bradford, M.M., *Anal. Biochem.* 72:248-254 (1976), which is incorporated herein by reference.

**[0104]** Binding assays are carried out in polypropylene tubes, each tube containing 0.5 ml of membrane suspension. 8 nM of 3H-[D-Ala<sup>2</sup>,Me-Phe<sup>4</sup>,Gly<sup>5</sup>]enkephalin (DAMGO) (specific activity = 36 Ci/mmol, 160,000 cpm per tube; which can be obtained from Multiple Peptide Systems, San Diego, CA, through NIDA drug distribution program 271-90-7302) and 80 µg/ml of bicyclic guanidine, individual or as a mixture and Tris-HCl buffer in a total volume of 0.65 ml. Assay tubes are incubated for 60 mins. at 25°C. The reaction is terminated by filtration through GF-B filters on a Tomtec harvester (Orange, CT). The filters are

subsequently washed with 6 ml of Tris-HCl buffer, 4°C. Bound radioactivity is counted on a Pharmacia Biotech Betaplate Liquid Scintillation Counter (Piscataway, NJ) and expressed in cpm. To determine inter- and intra-assay variation, standard curves in which 3H-DAMGO is incubated in the presence of a range of concentrations of unlabeled DAMGO (0.13-3900 nM) are generally included in each plate of each assay (a 96-well format). Competitive inhibition assays are performed as above using serial dilutions of the piperidine-3-carboxamides, individually or in mixtures. IC<sub>50</sub> values (the concentration necessary to inhibit 50% of 3H-DAMGO binding) are then calculated. IC<sub>50</sub> values of less than 1000 nM are indicative of highly active opioid compounds which bind to the  $\mu$  receptor, with particularly active compounds having IC<sub>50</sub> values of 100 nM or less and the most active compounds with values of less than 10 nM.

**[0105]** As opposed to this  $\mu$  receptor selective assay, which can be carried out using 3H-DAMGO as radioligand, as described above, assays selective for  $\kappa$  receptors can be carried out using [3H]-U69,593 (3 nM, specific activity 62 Ci/mmol) as radioligand. Assays selective for  $\delta$  opiate receptors can be carried out using tritiated DSLET ([D-Ser2, D-Leu5]-threonine-enkephalin) as radioligand. Assays selective for the  $\sigma$  opiate receptor can use radiolabeled pentazocine as ligand.

**[0106]** Screening of combinatorial libraries and compounds of the invention can be done with an anti-fungal assay. Compounds of the present invention can be useful for treating fungal infections.

**[0107]** Screening of combinatorial libraries and compounds of the invention also can be done with a calmodulin-dependent phosphodiesterase (CaMPDE) assay. Compounds of the present invention can be useful as calmodulin antagonists.

**[0108]** Calmodulin (CaM), which is the major intracellular calcium receptor, is involved in many processes that are crucial to cellular viability. In particular, calmodulin is implicated in calcium-stimulated cell proliferation. Calmodulin

antagonists are, therefore, useful for treating conditions associated with increased cell proliferation, for example, cancer. In addition, calmodulin antagonists such as compounds of the subject invention are useful both in vitro and in vivo for identifying the role of calmodulin in other biological processes. The disadvantages of known antagonists such as trifluoperazine and N-(4-aminobutyl)-5-chloro-2-naphthalenesulfonamide (W13) include their non-specificity and toxicity. In contrast, advantages of the combinatorial libraries and compounds of the subject invention as calmodulin antagonists include their reduced flexibility and ability to generate broader conformational space of interactive residues as compared to their linear counterparts.

**[0109]** An example of an assay that identifies CaM antagonists is a CaMPDE assay. In brief, samples are mixed with 50  $\mu$ l of assay buffer (360 mM Tris, 360 mM Imidazole, 45 mM Mg(CH<sub>3</sub>COO)<sub>2</sub>, pH 7.5) and 10  $\mu$ l of CaCl<sub>2</sub> (4.5 mM) to a final volume of 251  $\mu$ l. 25  $\mu$ l of calmodulin stock solution (Boehringer Mannheim; 0.01  $\mu$ g/ $\mu$ l) is then added and the samples then sit at room temperature for 10 minutes. 14  $\mu$ l of PDE (Sigma; 2 Units dissolved in 4 ml of water; stock concentration: 0.0005 Units/ $\mu$ l) is then added, followed by 50  $\mu$ l of 5'-nucleotidase (Sigma; 100 Units dissolved in 10 ml of 10 mM Tris-HCl containing 0.5 mM Mg(CH<sub>3</sub>COO)<sub>2</sub>, pH 7.0; stock concentration: 10 Units/ml). The samples are then incubated for 10 minutes at 30°C. 50  $\mu$ l of adenosine 3',5'-cyclic monophosphate (cAMP) (20 mM in water at pH 7.0) is added, the samples incubated for 1 hour at 30°C and then vortexed. 200  $\mu$ l of trichloroacetic acid (TCA) (55% in water) is added to a 200  $\mu$ l sample aliquot, which is then vortexed and centrifuged for 10 minutes. 80  $\mu$ l of the resulting supernatants of each sample is transferred to a 96-well plate, with 2 wells each containing 80  $\mu$ l of each sample. 80  $\mu$ l of ammonium molybdate (1.1% in 1.1N H<sub>2</sub>SO<sub>4</sub>) is then added to all the wells, and the OD of each were determined at 730nm, with the values later subtracted to the final OD reading. 16  $\mu$ l of reducing agent (6g sodium bisulfite, 0.6g sodium sulfite and 125mg of 1-amino-2-naphtol-4-sulfonic acid in 50ml of water) is then added to one of each sample duplicate and 16  $\mu$ l of water is added to the other duplicate. After sitting for 1 hour at room

temperature, the OD of each well is determined at 730nm. The percent inhibition of calmodulin activity is then calculated for each sample, using as 0% inhibition a control sample containing all reagents without any test samples and as 100% inhibition a control sample containing test samples and all reagents except calmodulin. In addition, the percent inhibition of phosphodiesterase activity was determined by following a similar protocol as the CaMPDE assay described above, except not adding calmodulin to the sample mixture and calculating the percent inhibition by using as 0% inhibition a control reagent without any test samples and as 100% inhibition a control sample containing test samples and all reagents except cAMP.

**[0110]** The following examples are provided to illustrate but not limit the present invention. The following abbreviations have the corresponding meanings:

DMF : N,N-dimethylformamide;

HOBt : 1-hydroxybenzotriazole;

Boc : tert-butoxycarbonyl;

DIC : N,N--diisopropylcarbodiimide;

TFA : trifluoroacetic acid;

DIEA : N,N-diisopropylethylamine;

DCM : dichloromethane;

RT : room temperature

MeOH: methanol

MeOEtOH : 2-methoxyethanol

DCE : 1,2-dichloroethane

THF : tetrahydrofuran

ACN : acetonitrile

Wang resin : *p*-benzyloxybenzyl alcohol-polystyrene Br-Wang resin :

*p*-benzyloxybenzyl bromide-polystyrene

PP : polypropylene

PPh<sub>3</sub>Br<sub>2</sub> : triphenylphosphine dibromide

DMAP : 4-dimethylamino-pyridine

## Example 1

### Synthetic Protocol

#### Step 1a. Loading Hydroxybenzaldehydes on Bromo-Wang Resin

**[0111]** A 1 L Pyrex media bottle was charged with 100 g Bromo-Wang resin (100-200 mesh, 1.4 mmol/g). DMF (350 ml) was added and the bottle was shaken by hand to distribute the solvent within the swollen resin. A 500 ml Pyrex media bottle was charged with the hydroxybenzaldehyde (420 mmol, 3 eq) and the aldehyde was dissolved in DMF (300 ml). The aldehyde solution was cooled to 0° C (ice bath) and potassium *tert*-butoxide (44.8 g, 400 mmol) was added in two equal portions shaking for about 5 min. between additions. CAUTION: EXOTHERMIC REACTION. The temperature must be maintained at or below 25° C. The bottle was removed from the ice bath and shaken periodically to help dissolve the potassium *tert*-butoxide completely. After the second portion of potassium *tert*-butoxide was added, the bottle was allowed to warm to 25° C. After 30 min. at 25° C, all the potassium *tert*-butoxide dissolved and the solutions had various dark colors. The phenoxide solution was added to the swollen resin in two portions, shaking between portions. The 1L bottles were clamped horizontally in an orbital shaker oven and allowed to shake at 25° C for 30 min. The temperature was then increased to 50° C and the reaction allowed to shake for 14 h. After cooling, each resin slurry was poured into a 8" x 10" 3-sided porous polypropylene packet (tea bag) sitting in a 2 L beaker. After the solvent mixture had drained from the resin, the fourth side of the tea bag was sealed and the tea bags were washed in wide-mouth HDPE Nalgene bottles as follows: 2 x DMF, 4 x DMF/H<sub>2</sub>O (4:1), 3 x DMF, 4 x MeOH. The tea bags were allowed to air dry in a fume hood.

#### Step 1b. Loading Diamines on Wang-Imidazolid Resin

**[0112]** For each R<sub>1</sub> diamine, a 4 L Nalgene bottle was charged with 17 x 2.5 g



tea bags containing Wang resin (100-200 mesh, 1.4 mmol/g). DCM (2 L) was added followed by 1,1'-carbonyldiimidazole (97 g, 0.60 mol, 0.3 M). The bags were shaken for 3 h at room temperature. Each diamine (0.72 mol, 0.4 M) was placed in a 2 L Nalgene bottle and 1.8 L of DCM added.

**[0113]** After 3 h shaking with CDI, the Wang-imidazolidine tea bags were washed quickly with DCM (x2). The diamine solution was added immediately and the bags shaken overnight at room temperature. The bags were washed with DCM (x3) and MeOH (x3).

#### **Step 2a. Imine Formation for the R<sub>1</sub> Hydroxybenzaldehydes.**

**[0114]** After splitting the tea bags from step 1a, each set of 8 x 2.5 g bags was placed into a 1 L Nalgene bottle. The containers were then filled with 250 ml of trimethylorthoformate and 250 ml of anhydrous DMF. After the bags were saturated with the solvent, the primary amine (150 mmol, 0.3 M) was added. The reaction was then allowed to shake at room temperature for 24 h. The wash procedure must be carried out just before step 3 and the description is included in that section.

#### **Step 2b. Imine Formation for the R<sub>1</sub> Primary Diamines.**

**[0115]** After splitting the tea bags from step 1b, each set of 7 x 2.5 g bags was placed into a 1 L Nalgene bottle. The containers were then filled with 250 ml of trimethylorthoformate and 250 ml of anhydrous DMF. After the bags were saturated with the solvent, the aldehyde (150 mmol, 0.3 M) was added. The reaction was then shaken at room temperature for 24 h. The wash procedure must be carried out just before step 3 and is described in that section.

#### **Step 3. Cyclization with 2-Phenylglutaric Anhydride**

**[0116]** In an 8L Nalgene bottle, 2-Phenylglutaric anhydride (1.0 mol, 0.4M) was completely dissolved in 2.5L anhydrous DMF and triethylamine (0.03 M) was added. This anhydride solution is created before washing the imine tea bags. The imine tea bags from step 2 (60 X 2.5g bags) were quickly washed with

anhydrous DMF (3 x, 3 minutes or less washing). After washing, the imine bags were immediately transferred to the 2-Phenylglutaric anhydride solution and the reaction shaken at RT for 5 days. The bags were washed with DMF (x3) DCM (x3) and MeOH (x3) and air-dried.

#### **Step 4. Acylation of the Resin Bound Carboxylic Acid.**

**[0117]** Each tea bag from step 3 was plated into 40 wells of a 2 ml deep-well microtiter plate. The resin bound carboxylic acid was pre-activated by treatment with 0.6 ml of a solution containing 0.6 M DIC, 0.6M HOBt in anhydrous DMF. The plates were allowed to stand for one hour at room temperature. During this time, each amine solution was prepared by dissolving the amine (0.6M) in a solution of DIEA (0.8 M) in DMF. To each well containing the pre-activated acid resin was added 0.6 ml of the amine solution. The final concentrations in each well were: amine (0.3M), DIEA (0.4 M), HOBt (0.3 M), and DIC (0.3 M). The plates were vortexed and were placed in a shaker oven at 50° C for 24 h. After cooling to room temperature, the resin was washed using a robotic wash station with 20% water/DMF (x2), DMF (x8) and MeOH (x6) and air-dried.

#### **Step 5. Cleavage from Linker and Extraction**

**[0118]** To dry microtiter plates was added 0.5 ml of 20% TFA/DCM to each well. The plates were capped and placed on a shaker at room temperature for 2 h. The plates were transferred to a GENEVAC to remove the volatile TFA/DCM solution. The resin was extracted with AcOH and the extracts were frozen and lyophilized to afford the products as yellow oils. All of the final products were analyzed by HPLC/MS using ELSD detection to determine purity.

### **Example 2**

#### **Preparation of (Substituted Phenyl)-glutaric anhydrides**

**[0119]** The appropriate substituted phenylacetic acid ethyl or methyl ester **1** (0.01 mol) is dissolved in anhydrous ethanol (100 ml). To this solution is added

Sodium ethoxide (0.01 mol), followed by ethyl acrylate (0.015 mol), and the solution is heated to reflux overnight. The solution is cooled and the solvent evaporated under reduced pressure. The product **2** is then dissolved in 100 ml H<sub>2</sub>O/EtOH 1:1 and KOH added (0.10 mol). The solution is heated to reflux for 10 hours, acidified to pH 3 with 1 N HCl and the diacid product **3** extracted with EtOAc, washed with water and brine, and dried with MgSO<sub>4</sub>. After removal of the solvent, the resulting solid is suspended in Acetic anhydride (100 ml) and heated to reflux for 1 hour to afford the anhydride. The solvent is removed and the residue is suspended in toluene and evaporated to afford the product **4**.

List of Compounds **1**:

ETHYL 2-THIOPHENEACETATE  
 ETHYL THIOPHENE-3-ACETATE  
 INDOLE-3-ACETIC ACID ETHYL ESTER  
 ETHYL 2-PYRIDYLACETATE  
 ETHYL 3-PYRIDYLACETATE  
 ETHYL O-TOLYLACETATE  
 ETHYL P-TOLYLACETATE  
 METHYL 1-METHYL-2-PYRROLEACETATE  
 METHYL 2,3,4,5,6-PENTAFLUOROPHENYLACETATE  
 ETHYL 2-NAPHTHYLACETATE  
 METHYL 2-(4,5-DIMETHOXY-2-NITROPHENYL)ACETATE  
 ETHYL P-BROMOPHENYLACETATE  
 ETHYL 4-NITROPHENYLACETATE  
 METHYL 2,3,4-TRIMETHOXYPHENYL ACETATE  
 METHYL 3,4,5-TRIMETHOXYPHENYL ACETATE  
 ETHYL 3,4-DIMETHOXYPHENYLACETATE  
 ETHYL M-TOLYLACETATE  
 2,4-DICHLOROPHENYLACETIC ACID METHYL ESTER  
 ETHYL 4-CHLOROPHENYLACETATE  
 ETHYL 1-NAPHTHYLACETATE  
 ETHYL 3-METHOXYPHENYLACETATE  
 ETHYL 4-BENZYLOXYPHENYLACETATE  
 ETHYL 4-METHOXYPHENYLACETATE  
 5-BENZYLOXYINDOLE-3-ACETIC ACID METHYL ESTER  
 ETHYL PYRIDINE-4-ACETATE  
 METHYL 4-TERT-BUTYLPHENYLACETATE  
 ETHYL MESITYLACETATE  
 ETHYL 4-ETHOXYPHENYLACETATE  
 ETHYL 2-BROMOPHENYLACETATE  
 4-BUTOXYPHENYLACETIC ACID METHYL ESTER

ETHYL 3,5-DIMETHYLPHENYLACETATE  
 METHYL 3,5-DIMETHOXYPHENYLACETATE  
 ETHYL 2-NITROPHENYLACETATE  
 2-CHLOROPHENYLACETIC ACID METHYL ESTER  
 METHYL 4-BENZYLOXYPHENYLACETATE  
 METHYL 5-CHLOROBENZO[B]THIEN-3-YLACETATE  
 2,6-DICHLOROPHENYLACETIC ACID METHYL ESTER  
 ETHYL 2,5-DIMETHOXYPHENYLACETATE  
 METHYL (5-METHYL-2-PHENYLOXAZOL-4-YL)ACETATE  
 METHYL 5,6-DICHLORO-3-INDOLEACETATE  
 METHYL 2-(5-METHOXY-2-METHYL-1H-INDOL-3-YL)ACETATE  
 METHYL (5-METHYL-2-PHENYLTHIAZOL-4-YL)ACETATE  
 IMIDAZO(2,1-B)THIAZOL-6-YL-ACETIC ACID ETHYL ESTER  
 (4-CHLORO-2-NITRO-PHENYL)-ACETIC ACID ETHYL ESTER  
 ETHYL 2-(TRIFLUOROMETHYL)PHENYL ACETATE  
 ETHYL 2-[2-(ACETYLAMINO)-1,3-THIAZOL-4-YL]ACETATE  
 (1H-IMIDAZOL-4-YL)-ACETIC ACID METHYL ESTER  
 (4,5-DIMETHOXY-2-NITRO-PHENYL)-ACETIC ACID ETHYL ESTER  
 ETHYLFURYL ACETATE  
 METHYL 2-FLUOROPHENYLACETATE  
 METHYL 2-CHLORO-6-FLUOROPHENYLACETATE  
 METHYL 4-FLUOROPHENYLACETATE  
 METHYL 2-CHLORO-4-FLUOROPHENYL ACETATE  
 METHYL 3-CHLOROPHENYLACETATE  
 METHYL 3,4-DICHLOROPHENYLACETATE  
 ETHYL 2-(2-PHENYL-1,3-THIAZOL-4-YL)ACETATE  
 ETHYL 3,4-DICHLOROPHENYLACETATE  
 ETHYL 2-(2-METHYL-1,3-THIAZOL-4-YL)ACETATE  
 ETHYL 2-[2-[4-(TERT-BUTYL)PHENYL]-1,3-THIAZOL-4-YL]ACETATE  
 ETHYL 2-[2-(4-CHLOROPHENYL)-1,3-THIAZOL-4-YL]ACETATE  
 METHYL (2-CYANOPHENYL)ACETATE  
 METHYL (4-CYANOPHENYL)ACETATE

### Example 3

#### Anti-microbial Screen

**[0120]** *Streptococcus pyogenes* (ATCC# 97-03 14289) was grown in Todd Hewitt Broth (THB) (Difco Laboratories #0492-17-6) overnight until reaching an optical density of ( OD = 0.636@ 570 nm) by reading 0.1 ml in a 96 well microtiter plate in a Molecular Devices Thermomax. This preparation was kept frozen as stocks in 30% v/v glycerol in 1.5 ml aliquots at -70mC until use. Prior to experiments, 6 ml aliquots were thawed and diluted into 50 ml 2X THB. 60 ul

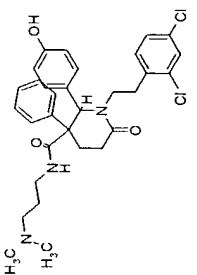
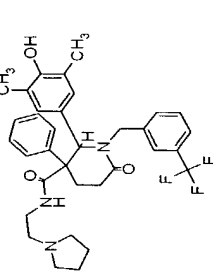
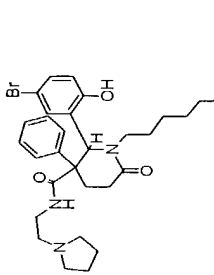
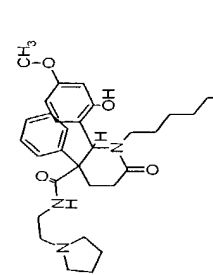
of this dilution was added to 92 wells of microtiter plate. To three wells THB (200 ul) was added to serve as a blank and a sterility control. Test compounds in DMSO and appropriate concentrations of DMSO were added to Growth/Solvent Controls at 0 time. Plates were read at 0 time at 570 nm in the Molecular Devices plate reader to obtain compounds correction factors for insoluble or colored compounds. Plates were read again at 4 hours.

**[0121]** Percent inhibition is calculated with the following formula

**[0122]** Color correct = O.D. 0 hr - Blank 0 hr)-(Solvent Control 0hr - Blank 0 hr)

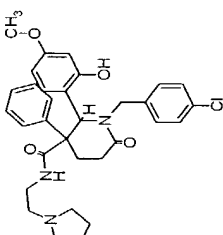
**[0123]** % Inhibition =

100 - O.D. test compound 4 hr - Blank 4 hr - color correct O.D. growth/solvent control 4 hr - Blank 4 hr

Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	Lion ID	#NAME?	Chemical Structure	Molecular Formula	Mass
9100	2979	1	000728122	9100-042	C 04	0.098	99.97	Spy4H	0.1776	TR0910002979	0.1776	TR0910002979	?		C <sub>31</sub> H <sub>35</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	568 542
9100	682	1	000726065	9100-009	B 07	0.112	98.90	Spy4H	0.1776	TR0910000682	0.1776	TR0910000682	?		C <sub>24</sub> H <sub>38</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	593.686
9100	2442	1	000727585	9100-035	B 07	0.17	97.52	Spy4H	0.1776	TR0910002442	0.1776	TR0910002442	?		C <sub>30</sub> H <sub>40</sub> Br N <sub>3</sub> O <sub>3</sub>	570 568
9100	3002	1	000728145	9100-042	B 07	0.112	97.51	Spy4H	0.1776	TR0910003002	0.1776	TR0910003002	?		C <sub>31</sub> H <sub>43</sub> N <sub>3</sub> O <sub>4</sub>	521 698

ADONIS-094666

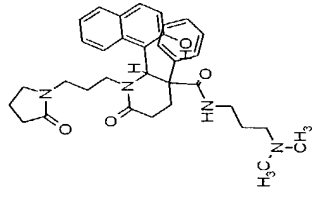


Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc.mg/ml	LionID	#NAME?	Chemical Structure	Formula	MW
9100	2722	1	000727865	9100-035	B 02	0.112	95.57	Spy4H	0.1776	TR0910002722	#NAME?		C <sub>32</sub> H <sub>36</sub> Cl N <sub>3</sub> O <sub>4</sub>	562.106
9100	2449	1	000727592	9100-035	A 08	0.216	95.27	Spy4H	0.1776	TR0910002449	#NAME?		C <sub>29</sub> H <sub>38</sub> Br N <sub>3</sub> O <sub>3</sub>	556.541
9100	2467	1	000727610	9100-035	C 10	0.234	94.31	Spy4H	0.1776	TR0910002467	#NAME?		C <sub>27</sub> H <sub>35</sub> Br N <sub>2</sub> O <sub>4</sub>	531.487

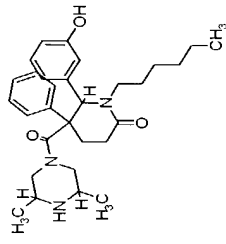
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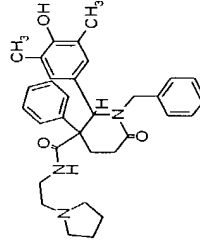
Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>34</sub> H <sub>42</sub> N <sub>4</sub> O <sub>4</sub>	570.73
9100	3739	1	000728882	9100-051	C 09	0 132	94.27	Spy4H	0.1776	TR0910003739			



9100	1029	1	000726412	9100-013	E 10	0.162	94.11	Spy4H	0.1776	TR0910001029	#NAME?	C <sub>30</sub> H <sub>41</sub> N <sub>3</sub> O <sub>3</sub>	491.672
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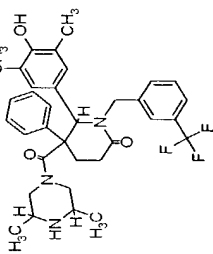
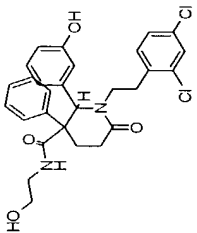
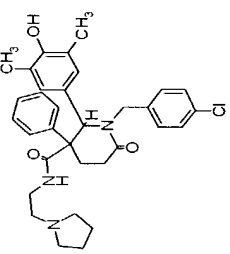
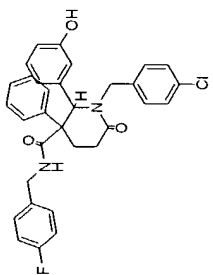


9100	2402	1	000727545	9100-035	B 02	0.12	92.38	Spy4H	0.1776	TR0910002402	#NAME?	C <sub>33</sub> H <sub>39</sub> N <sub>3</sub> O <sub>3</sub>	525.689
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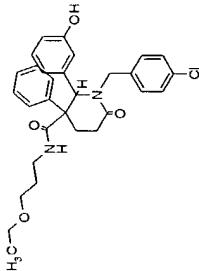
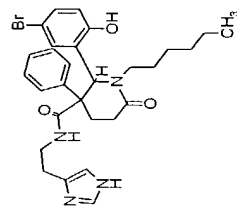
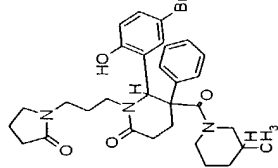
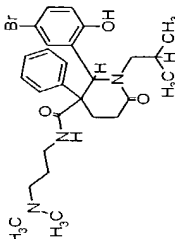


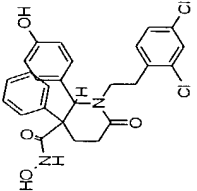
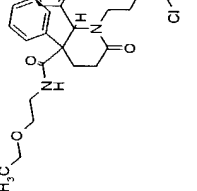
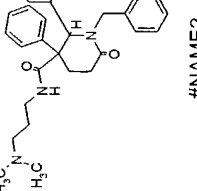
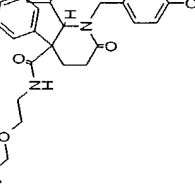
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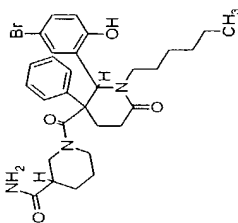
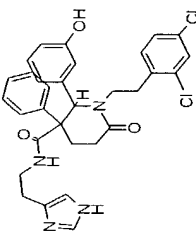
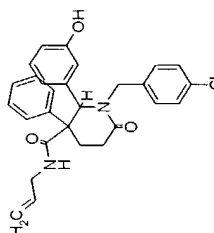
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9100	709	1	000726092	9100-009	E 10	0.178	83.73	Spy4H	0.1776	TR0910000709					C <sub>34</sub> H <sub>38</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	593.686
9100	657	1	000726040	9100-009	A 04	0.188	83.39	Spy4H	0.1776	TR0910000657					C <sub>28</sub> H <sub>28</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>	527.445
9100	2602	1	000727745	9100-037	B 07	0.157	83.27	Spy4H	0.1776	TR0910002602					C <sub>33</sub> H <sub>38</sub> Cl N <sub>3</sub> O <sub>3</sub>	560.134
9100	853	1	000726236	9100-011	E 08	0.28	83.27	Spy4H	0.1776	TR0910000853					C <sub>32</sub> H <sub>28</sub> Cl F N <sub>2</sub> O <sub>3</sub>	543.035

ADAMANTO # 624444

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?		Formula	MW
9100	862	1	000726245	9100-011	F 09	0.255	83.27	Spy4H	0.1776	0.1776	TR0910000862	TR0910000862	C <sub>30</sub> H <sub>33</sub> Cl N <sub>2</sub> O <sub>4</sub>		521.054	
9100	2444	1	000727587	9100-035	D 07	0.275	82.77	Spy4H	0.1776	0.1776	TR0910002444	TR0910002444	C <sub>29</sub> H <sub>35</sub> Br N <sub>4</sub> O <sub>3</sub>		567.524	
9100	995	1	000726378	9100-013	C 06	0.291	82.45	Spy4H	0.1776	0.1776	TR0910000995	TR0910000995	C <sub>31</sub> H <sub>35</sub> Br N <sub>3</sub> O <sub>4</sub>		596.562	
9100	1699	1	000726842	9100-023	C 04	0.177	82.26	Spy4H	0.1776	0.1776	TR0910001699	TR0910001699	C <sub>27</sub> H <sub>36</sub> Br N <sub>3</sub> O <sub>3</sub>		530.503	

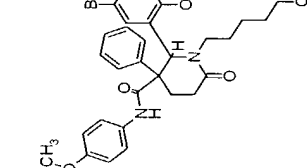
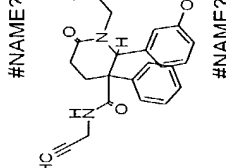
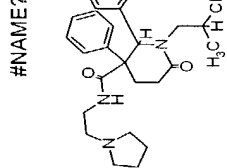
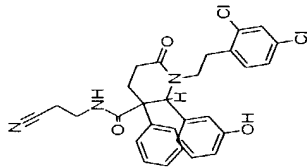
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9100	2997	1	000728140	9100-042	E 06	0.488	82.26	Spy4H	0.1776	TR0910002997			
9100	668	1	000726051	9100-009	D 05	0.328	82.04	Spy4H	0.1776	TR0910000668		C <sub>30</sub> H <sub>32</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>	555.499
9100	2419	1	000727562	9100-035	C 04	0.157	81.80	Spy4H	0.1776	TR0910002419		C <sub>32</sub> H <sub>39</sub> N <sub>3</sub> O <sub>3</sub>	513.678
9100	868	1	000726251	9100-011	D 10	0.248	81.37	Spy4H	0.1776	TR0910000868		C <sub>29</sub> H <sub>31</sub> ClN <sub>2</sub> O <sub>4</sub>	507.027

499 392 555.499 513.678 507.027

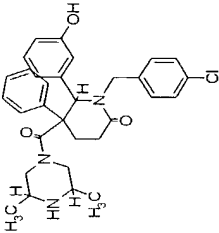
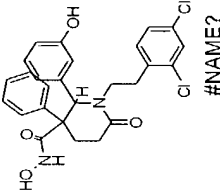
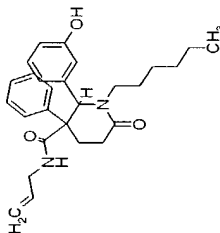
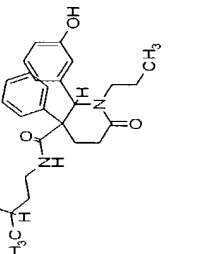
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>30</sub> H <sub>38</sub> Br N <sub>3</sub> O <sub>4</sub>	584.551
9100	2441	1	000727584	9100-035	A 07	0.199	79.88	Spy4H	0.1776	TR0910002441			
9100	644	1	000726027	9100-009	D 02	0.211	78.67	Spy4H	0.1776	TR0910000644		C <sub>31</sub> H <sub>30</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>3</sub>	577.509
9100	846	1	000726229	9100-011	F 07	0.31	78.13	Spy4H	0.1776	TR0910000846		C <sub>28</sub> H <sub>27</sub> Cl N <sub>2</sub> O <sub>3</sub>	474.985

46994695 060322

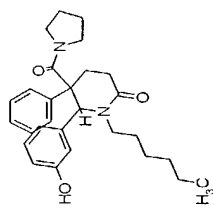
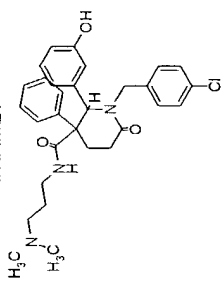
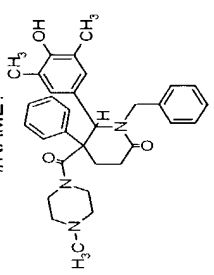
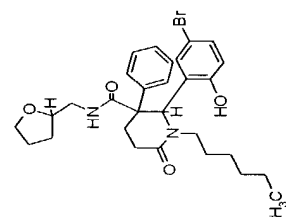
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9100	674	1	000726057	9100-009	B 06	0 275	77 32	Spy4H	0 1776	TR0910000674			
9100	1682	1	000726825	9100-023	B 02	0 193	77.18	Spy4H	0 1776	TR0910001682			
9100	870	1	000726253	9100-011	F 10	0 278	76 50	Spy4H	0 1776	TR0910000870			
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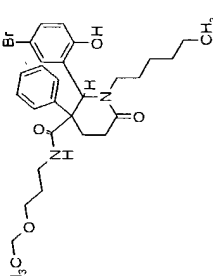
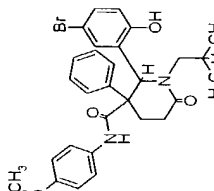
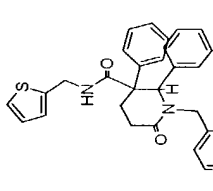
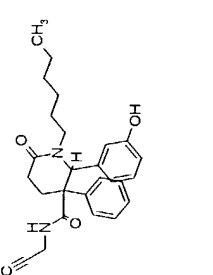


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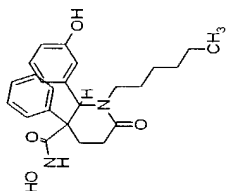
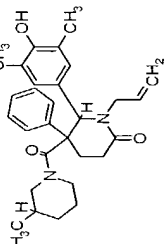
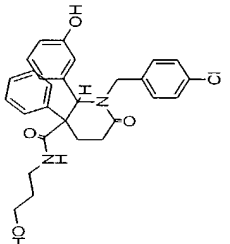
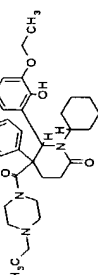
Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	C <sub>31</sub> H <sub>34</sub> Cl N <sub>3</sub> O <sub>3</sub>	532.081
9100	869	1	000726252	9100-011	E 10	0.255	75.69	Spy4H	0.1776	TR0910000869					
9100	677	1	000726060	9100-009	E 06	0.23	75.63	Spy4H	0.1776	TR0910000677					
9100	1006	1	000726389	9100-013	F 07	0.334	75.14	Spy4H	0.1776	TR0910001006					
9100	1101	1	000726484	9100-014	E 09	0.263	74.29	Spy4H	0.1776	TR0910001101					



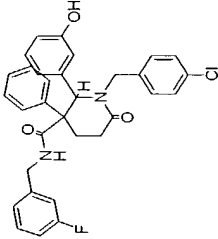
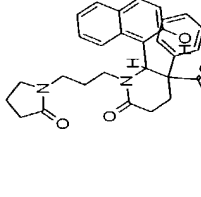
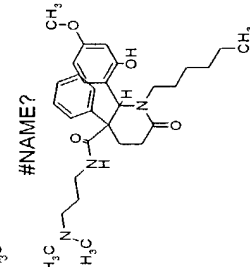
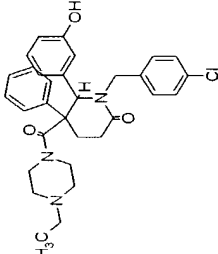
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9100	1003	1	000726386	9100-013	C 07	0.302	74.05	Spy4H	0.1776	TR0910001003				
9100	859	1	000726242	9100-011	C 09	0.204	73.80	Spy4H	0.1776	TR0910000859			C <sub>30</sub> H <sub>34</sub> Cl N <sub>3</sub> O <sub>3</sub>	520.07
9100	2409	1	000727552	9100-035	A 03	0.211	73.79	Spy4H	0.1776	TR0910002409			C <sub>32</sub> H <sub>37</sub> N <sub>3</sub> O <sub>3</sub>	511.662
9100	2450	1	000727593	9100-035	B 08	0.294	73.79	Spy4H	0.1776	TR0910002450			C <sub>29</sub> H <sub>37</sub> Br N <sub>2</sub> O <sub>4</sub>	557.525

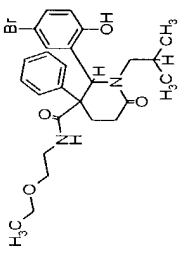
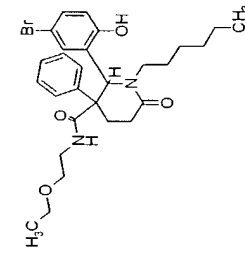
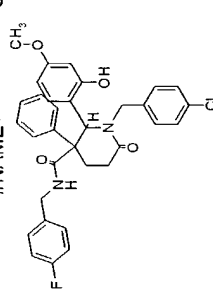
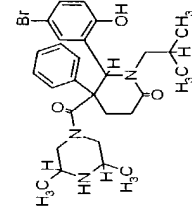
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9100	1716	1	000726859	9100-023	D 06	0.445	73.16	Spy4H	0.1776	TR0910001716	TR0910001716	#NAME?		C <sub>29</sub> H <sub>31</sub> Br N <sub>2</sub> O <sub>4</sub>	551.478
9100	858	1	000726241	9100-011	B 09	0.303	72.99	Spy4H	0.1776	TR0910000858	TR0910000858	#NAME?		C <sub>30</sub> H <sub>27</sub> Cl N <sub>2</sub> O <sub>3</sub> S	531.073
9100	1030	1	000726413	9100-013	F 10	0.28	72.97	Spy4H	0.1776	TR0910001030	TR0910001030	#NAME?		C <sub>27</sub> H <sub>32</sub> N <sub>2</sub> O <sub>3</sub>	432.561

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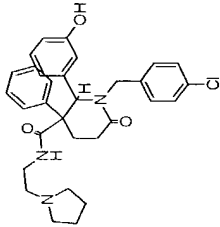
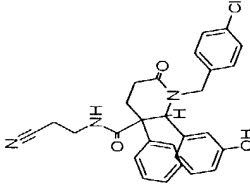
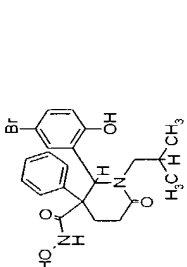
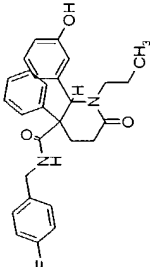
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9100	1037	1	000726420	9100-013	E 11	0.26	72.97	Spy4H	0.1776	TR0910001037				C <sub>24</sub> H <sub>30</sub> N <sub>2</sub> O <sub>4</sub>	410.511
9100	1075	1	000726458	9100-014	C 06	0.3	72.88	Spy4H	0.1776	TR0910001075				C <sub>29</sub> H <sub>36</sub> N <sub>2</sub> O <sub>3</sub>	460.614
9100	867	1	000726250	9100-011	C 10	0.233	72.72	Spy4H	0.1776	TR0910000867				C <sub>28</sub> H <sub>29</sub> Cl N <sub>2</sub> O <sub>4</sub>	493
9100	2340	1	000727483	9100-033	D 04	0.216	72.56	Spy4H	0.1776	TR0910002340				C <sub>32</sub> H <sub>43</sub> N <sub>3</sub> O <sub>4</sub>	533.709

40924905 : 020002

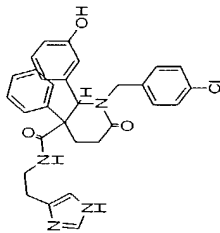
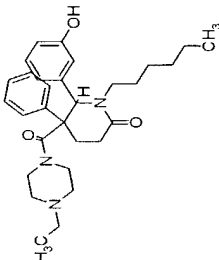
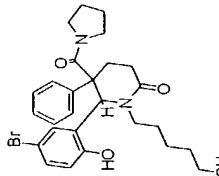
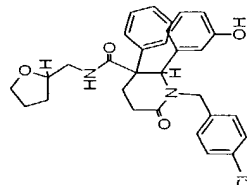
Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	Chemical Structure	Formula	Mass
9100	852	1	000726235	9100-011	D 08	0.332	72.45	Spy4H	0.1776	TR0910000852			C <sub>32</sub> H <sub>28</sub> Cl F N <sub>2</sub> O <sub>3</sub>	543.035
9100	3731	1	000728874	9100-051	C 08	0.3	72.29	Spy4H	0.1776	TR0910003731			C <sub>37</sub> H <sub>39</sub> N <sub>3</sub> O <sub>4</sub>	589.732
9100	3019	1	000728162	9100-042	C 09	0.205	72.18	Spy4H	0.1776	TR0910003019			C <sub>30</sub> H <sub>43</sub> N <sub>3</sub> O <sub>4</sub>	509.687
9100	860	1	000726243	9100-011	D 09	0.266	72.18	Spy4H	0.1776	TR0910000860			C <sub>31</sub> H <sub>34</sub> Cl N <sub>3</sub> O <sub>3</sub>	532.081

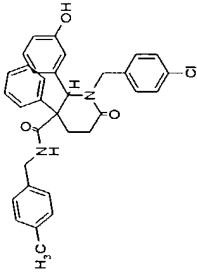
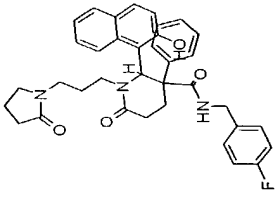
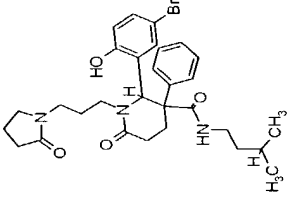
Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?			
9100	1708	1	000726851	9100-023	D 05	0 379	72 09	Spy4H	0 1776	TR0910001708				C <sub>26</sub> H <sub>33</sub> Br N <sub>2</sub> O <sub>4</sub>	517.461	
9100	2468	1	000727611	9100-035	D 10	0 28	71.54	Spy4H	0 1776	TR0910002468				C <sub>28</sub> H <sub>37</sub> Br N <sub>2</sub> O <sub>4</sub>	545.514	
9100	2733	1	000727876	9100-039	E 03	0 429	71 19	Spy4H	0 1776	TR0910002733				C <sub>33</sub> H <sub>30</sub> Cl F N <sub>2</sub> O <sub>4</sub>	573.061	
9100	1709	1	000726852	9100-023	E 05	0 383	71.02	Spy4H	0 1776	TR0910001709				C <sub>28</sub> H <sub>36</sub> Br N <sub>3</sub> O <sub>3</sub>	542.514	

40694292 # 00000000

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>31</sub> H <sub>34</sub> Cl N <sub>3</sub> O <sub>3</sub>	532.081
9100	842	1	000726225	9100-011	B 07	70.82	Spy4H	0.1776	TR0910000842					
9100	874	1	000726257	9100-011	B 11	70.82	Spy4H	0.1776	TR0910000874				C <sub>28</sub> H <sub>26</sub> Cl N <sub>3</sub> O <sub>3</sub>	487.984
9100	1717	1	000726860	9100-023	E 06	70.21	Spy4H	0.1776	TR0910001717				C <sub>22</sub> H <sub>25</sub> Br N <sub>2</sub> O <sub>4</sub>	461.353
9100	1093	1	000726476	9100-014	E 08	70.04	Spy4H	0.1776	TR0910001093				C <sub>28</sub> H <sub>29</sub> F N <sub>2</sub> O <sub>3</sub>	460.546

CONFIDENTIAL

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>30</sub> H <sub>29</sub> Cl N <sub>4</sub> O <sub>3</sub>	529.037
9100	844	1	000726227	9100-011	D 07	0.221	69.74	Spy4H	0.1776	TR0910000844			
9100	1020	1	000726403	9100-013	D 09	0.217	69.72	Spy4H	0.1776	TR0910001020		C <sub>30</sub> H <sub>41</sub> N <sub>3</sub> O <sub>3</sub>	491.672
9100	2443	1	000727586	9100-035	C 07	0.383	69.62	Spy4H	0.1776	TR0910002443		C <sub>28</sub> H <sub>35</sub> Br N <sub>2</sub> O <sub>3</sub>	527.5
9100	850	1	000726233	9100-011	B 08	0.322	69.47	Spy4H	0.1776	TR0910000850		C <sub>30</sub> H <sub>31</sub> Cl N <sub>2</sub> O <sub>4</sub>	519.038

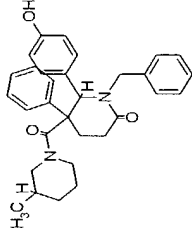
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc. mg/ml	LionID	#NAME?	Chemical Structure	Molecular Formula	Mass
9100	851	1	000726234	9100-011	C 08	0 374	69 20	Spy4H	0 1776	TR0910000851				C <sub>33</sub> H <sub>31</sub> Cl N <sub>2</sub> O <sub>3</sub>	539.072
9100	3733	1	000728876	9100-051	E 08	0 332	68 93	Spy4H	0 1776	TR0910003733				C <sub>35</sub> H <sub>36</sub> F N <sub>3</sub> O <sub>4</sub>	593.595
9100	981	1	000726364	9100-013	E 04	0 321	68 63	Spy4H	0 1776	TR0910000981				C <sub>30</sub> H <sub>33</sub> Br N <sub>3</sub> O <sub>4</sub>	584.551



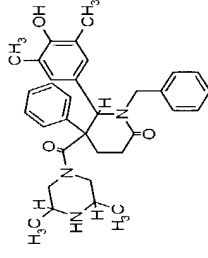


Library Cmpd Lot ExtReg Plate Well Raw Data Assay Result Assay Conc mg/ml LionID

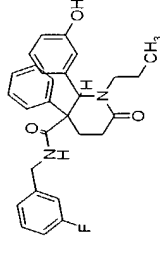
9100 1755 1 000726898 9100-023 C 11 0 363 67 80 Spy4H 0 1776 TR0910001755 C<sub>31</sub> H<sub>34</sub> N<sub>2</sub> O<sub>3</sub> 482.621



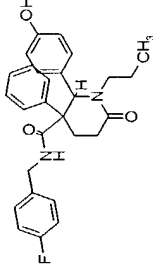
9100 2429 1 000727572 9100-035 E 05 0 217 67 70 Spy4H 0 1776 TR0910002429 C<sub>33</sub> H<sub>39</sub> N<sub>3</sub> O<sub>3</sub> 525.689



9100 1092 1 000726475 9100-014 D 08 0 322 67 49 Spy4H 0 1776 TR0910001092 C<sub>28</sub> H<sub>29</sub> F N<sub>2</sub> O<sub>3</sub> 460.546



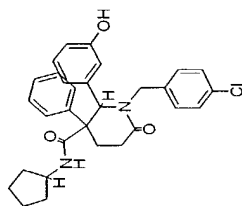
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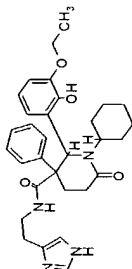
482.621 525.689 460.546 460.546

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID
9100	845	1	000726228	9100-011	E 07	0.421	67.31	Spy4H	0.1776	TR0910000845

#NAME? C<sub>30</sub> H<sub>31</sub> Cl N<sub>2</sub> O<sub>3</sub> 503 039

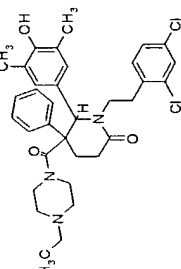


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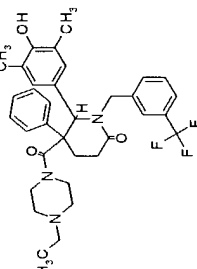
9100 2324 1 000727467 9100-033 D 02 0.232 66.94 Spy4H 0.1776 TR0910002324

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9100 2500 1 000727643 9100-036 D 04 0.388 66.93 Spy4H 0.1776 TR0910002500

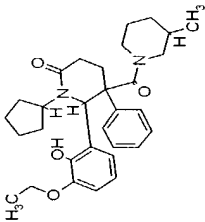
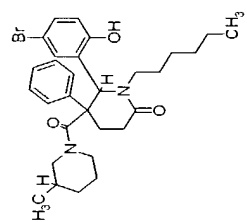
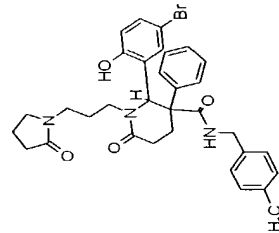
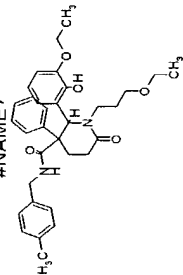
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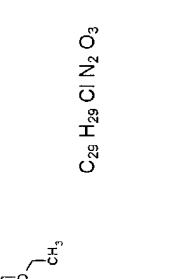

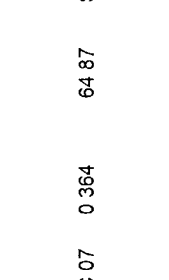
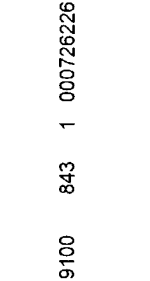
9100 700 1 000726083 9100-009 D 09 0.288 66.86 Spy4H 0.1776 TR0910000700

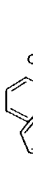





Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>31</sub> H <sub>40</sub> N <sub>2</sub> O <sub>4</sub>	504 667
9100	1955	1	000727098	9100-028	C 06	0 353	65.27	Spy4H	0 1776	TR0910001955				
9100	2475	1	000727618	9100-035	C 11	0 305	65 13	Spy4H	0 1776	TR0910002475			555 553	
9100	971	1	000726354	9100-013	C 03	0 379	65.11	Spy4H	0 1776	TR0910000971			618 568	
9100	2531	1	000727674	9100-036	C 08	0 302	65.06	Spy4H	0 1776	TR0910002531			544 688	

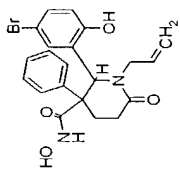
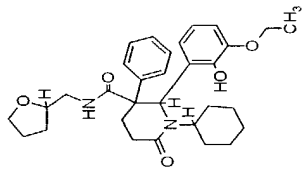
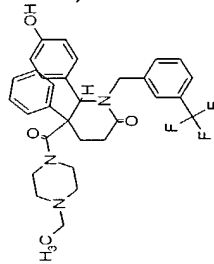
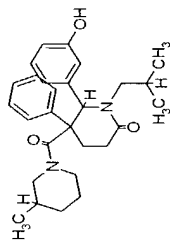
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Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID
9100	2533	1	000727676	9100-036	E 08	0.304	65.06	Spy4H	0.1776	0.1776	TR0910002533
<div>#NAME?</div> <div></div> <div>C<sub>32</sub>H<sub>37</sub>F N<sub>2</sub>O<sub>5</sub>      548.651</div>											
9100	843	1	000726226	9100-011	C 07	0.364	64.87	Spy4H	0.1776	0.1776	TR0910000843
<div>#NAME?</div> <div></div> <div>C<sub>29</sub>H<sub>29</sub>Cl N<sub>2</sub>O<sub>3</sub>      489.012</div>											
9100	2740	1	000727883	9100-039	D 04	0.384	64.80	Spy4H	0.1776	0.1776	TR0910002740
<div>#NAME?</div> <div></div> <div>C<sub>32</sub>H<sub>36</sub>Cl N<sub>3</sub>O<sub>4</sub>      562.106</div>											
9100	612	1	000725995	9100-008	D 08	0.339	64.80	Spy4H	0.1776	0.1776	TR0910000612
<div>#NAME?</div> <div></div> <div>C<sub>28</sub>H<sub>29</sub>F N<sub>2</sub>O<sub>3</sub>      460.546</div>											

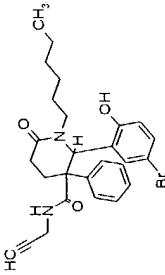
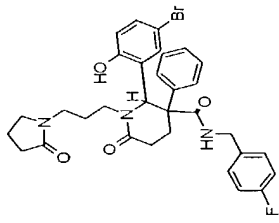
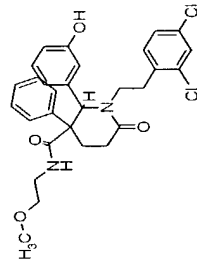
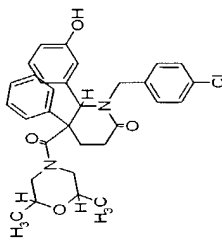
9100	843	1	000726226	9100-011	C 07	0 364	64 87	Spy4H	0.1776	TR0910000843	#NAME?		C <sub>28</sub> H <sub>29</sub> ClN <sub>2</sub> O <sub>3</sub>	489.012
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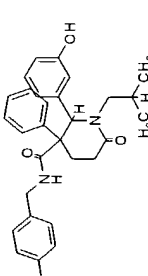
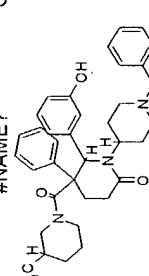
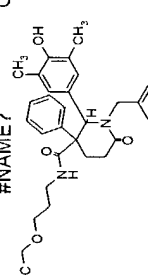
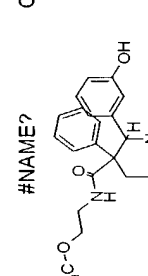
9100	2740	1	000727883	9100-039	D 04	0 384	64.80	Spv4H	0 1776	TR0910002740	#NAME?		C <sub>32</sub> H <sub>35</sub> Cl N <sub>3</sub> O <sub>4</sub>	562.106
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9100	612	1	000725995	9100-008	D 08	0.339	64.80	Spy4H	0.1776	TR0910000612	#NAME?		$C_{28}H_{25}F N_2 O_3$	460 546
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Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?				
9100	237	1	000725620	9100-003	E 11	0.281	Spy4H	64.74	0.1776	0.1776	TR0910000237	#NAME?		C <sub>21</sub> H <sub>21</sub> Br N <sub>2</sub> O <sub>4</sub>	445.311	
9100	2330	1	000727473	9100-033	B 03	0.281	Spy4H	64.69	0.1776	0.1776	TR0910002330	#NAME?		C <sub>31</sub> H <sub>40</sub> N <sub>2</sub> O <sub>5</sub>	520.666	
9100	4100	1	000729243	9100-057	D 04	0.261	Spy4H	64.67	0.1776	0.1776	TR0910004100	#NAME?		C <sub>32</sub> H <sub>34</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	565.633	
9100	595	1	000725978	9100-008	C 06	0.339	Spy4H	64.51	0.1776	0.1776	TR0910000595	#NAME?		C <sub>28</sub> H <sub>35</sub> N <sub>2</sub> O <sub>3</sub>	448.603	

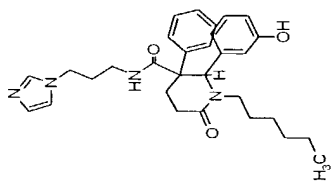


Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	
9100	2470	1	000727613	9100-035	F 10	0.294	64.49	Spy4H	0.1776	TR0910002470		C <sub>27</sub> H <sub>31</sub> Br N <sub>2</sub> O <sub>3</sub> 511.457
9100	973	1	000726356	9100-013	E 03	0.304	64.02	Spy4H	0.1776	TR0910000973		C <sub>32</sub> H <sub>33</sub> Br F N <sub>3</sub> O <sub>4</sub> 622.532
9100	647	1	000726030	9100-009	G 02	0.295	63.83	Spy4H	0.1776	TR0910000647		C <sub>29</sub> H <sub>30</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub> 541.472
9100	878	1	000726261	9100-011	F 11	0.356	63.79	Spy4H	0.1776	TR0910000878		C <sub>31</sub> H <sub>33</sub> Cl N <sub>2</sub> O <sub>4</sub> 533.065

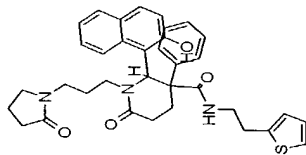
Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?		C <sub>29</sub> H <sub>31</sub> F N <sub>2</sub> O <sub>3</sub>	474.573
9100	573	1	000725956	9100-008	E 03	0.359	63.64	Spy4H	0.1776	TR0910000573	TR0910000573				
9100	2235	1	000727378	9100-031	C 11	0.239	63.59	Spy4H	0.1776	TR0910002235	TR0910002235	#NAME?		C <sub>36</sub> H <sub>43</sub> N <sub>3</sub> O <sub>3</sub>	565.754
9100	2422	1	000727565	9100-035	F 04	0.259	63.53	Spy4H	0.1776	TR0910002422	TR0910002422	#NAME?		C <sub>32</sub> H <sub>38</sub> N <sub>2</sub> O <sub>4</sub>	514.662
9100	847	1	000726230	9100-011	G 07	0.292	63.52	Spy4H	0.1776	TR0910000847	TR0910000847	#NAME?		C <sub>28</sub> H <sub>25</sub> Cl N <sub>2</sub> O <sub>4</sub>	493

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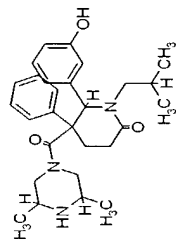
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9100	1014	1	000726397	9100-013	F 08	0.247	63.48	Spy4H	0.1776	TR0910001014								

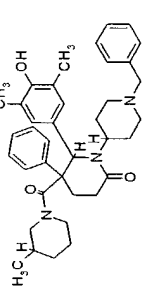
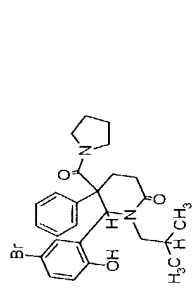
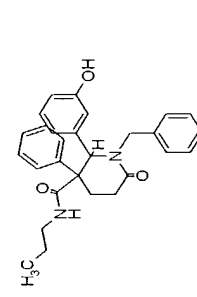
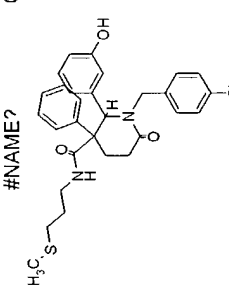


9100	3751	1	000728894	9100-051	G 10	0.289	63.44	Spy4H	0.1776	TR0910003751								595.76
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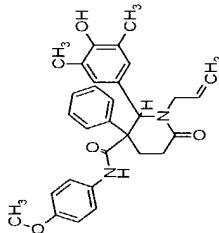
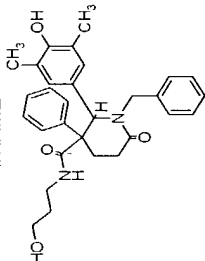
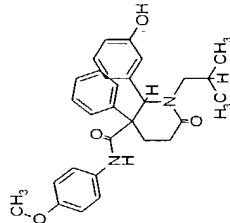
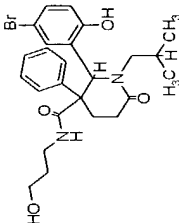


9100	589	1	000725972	9100-008	E 05	0.225	63.35	Spy4H	0.1776	TR0910000589								463.618
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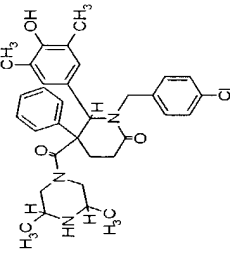
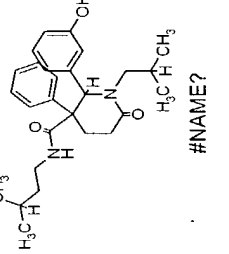
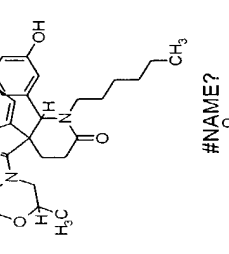
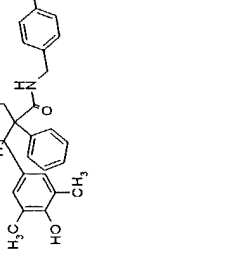


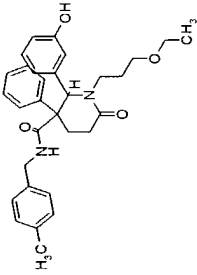
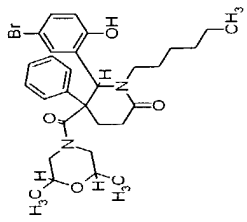
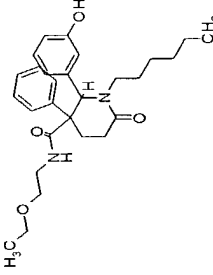
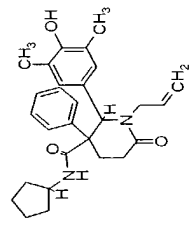
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9100	4155	1	000729298	9100-057	C 11	0.321	63.27	Spy4H	0.1776	0.1776	TR0910004155			C <sub>38</sub> H <sub>47</sub> N <sub>3</sub> O <sub>3</sub>	593.807	
9100	1683	1	000726826	9100-023	C 02	0.484	63.25	Spy4H	0.1776	0.1776	TR0910001683			C <sub>25</sub> H <sub>31</sub> Br N <sub>2</sub> O <sub>3</sub>	499.446	
9100	856	1	000726239	9100-011	H 08	0.335	63.25	Spy4H	0.1776	0.1776	TR0910000856			C <sub>29</sub> H <sub>29</sub> Cl N <sub>2</sub> O <sub>3</sub>	477.001	
9100	865	1	000726248	9100-011	A 10	0.272	63.25	Spy4H	0.1776	0.1776	TR0910000865			C <sub>29</sub> H <sub>31</sub> Cl N <sub>2</sub> O <sub>3</sub> S	523.094	

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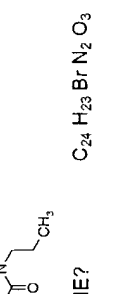

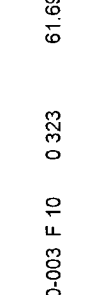
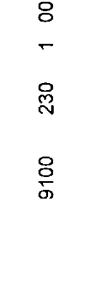
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	C <sub>30</sub> H <sub>32</sub> N <sub>2</sub> O <sub>4</sub>	484.593
9100	1076	1	000726459	9100-014	D 06	0.291	63.24	Spy4H	0.1776	TR0910001076					
9100	2427	1	000727570	9100-035	C 05	0.268	63.21	Spy4H	0.1776	TR0910002427				C <sub>30</sub> H <sub>34</sub> N <sub>2</sub> O <sub>4</sub>	486.609
9100	596	1	000725979	9100-008	D 06	0.286	63.06	Spy4H	0.1776	TR091000596				C <sub>29</sub> H <sub>32</sub> N <sub>2</sub> O <sub>4</sub>	472.582
9100	1707	1	000726850	9100-023	C 05	0.352	62.99	Spy4H	0.1776	TR0910001707				C <sub>25</sub> H <sub>31</sub> Br N <sub>2</sub> O <sub>4</sub>	503.434

484.593 = 66.609

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>33</sub> H <sub>38</sub> Cl N <sub>3</sub> O <sub>3</sub>	560.134
9100	2629	1	000727772	9100-037	E 10	0.275	62.89	Spy4H	0.1776	TR0910002629			
9100	581	1	000725964	9100-008	E 04	0.326	62.77	Spy4H	0.1776	TR0910000581		C <sub>27</sub> H <sub>36</sub> N <sub>2</sub> O <sub>3</sub>	436.592
9100	1038	1	000726421	9100-013	F 11	0.295	62.40	Spy4H	0.1776	TR0910001038		C <sub>30</sub> H <sub>40</sub> N <sub>2</sub> O <sub>4</sub>	492.656
9100	773	1	000726156	9100-010	E 08	0.231	62.39	Spy4H	0.1776	TR0910000773		C <sub>30</sub> H <sub>31</sub> F N <sub>2</sub> O <sub>3</sub>	486.584

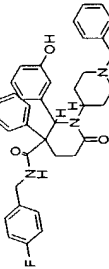
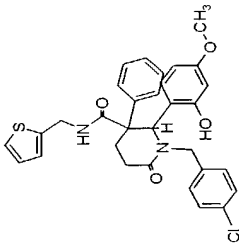
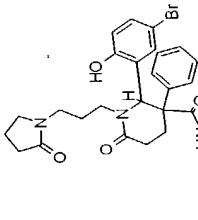
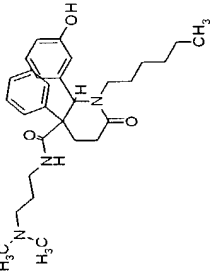
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9100	1971	1	000727114	9100-028	C 08	0.296	61.99	0.1776	Spv4H	0.1776	TR0910001971	
												#NAME?
												C <sub>31</sub> H <sub>38</sub> N <sub>2</sub> O <sub>4</sub>
												500.635
												
9100	2478	1	000727621	9100-035	F 11	0.265	61.92	0.1776	Spv4H	0.1776	TR0910002478	
												#NAME?
												C <sub>30</sub> H <sub>38</sub> Br N <sub>2</sub> O <sub>4</sub>
												571.552
												
9100	1028	1	000726411	9100-013	D 10	0.257	61.86	0.1776	Spv4H	0.1776	TR0910001028	
												#NAME?
												C <sub>28</sub> H <sub>38</sub> N <sub>2</sub> O <sub>4</sub>
												466.618
												
9100	1045	1	000726428	9100-014	E 02	0.331	61.83	0.1776	Spv4H	0.1776	TR0910001045	
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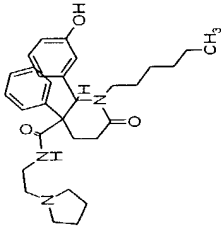
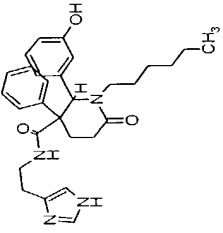
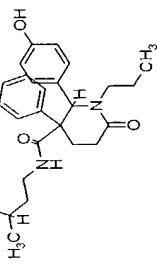
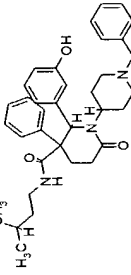
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9100	1091	1	000726474	9100-014	C 08	0.346	61.83	Sp4H	0.1776	TR0910001091	0.1776	456.583		C <sub>28</sub> H <sub>32</sub> N <sub>2</sub> O <sub>3</sub>	456.583	
9100	230	1	000725613	9100-003	F 10	0.323	61.69	Sp4H	0.1776	TR0910000230	0.1776	467.361		C <sub>24</sub> H <sub>23</sub> Br N <sub>2</sub> O <sub>3</sub>	467.361	
9100	855	1	000726238	9100-011	G 08	0.344	61.63	Sp4H	0.1776	TR0910000855	0.1776	474.985		C <sub>28</sub> H <sub>27</sub> Cl N <sub>2</sub> O <sub>3</sub>	474.985	
9100	3741	1	000728884	9100-051	E 09	0.246	61.60	Sp4H	0.1776	TR0910003741	0.1776	555.715		C <sub>34</sub> H <sub>41</sub> N <sub>3</sub> O <sub>4</sub>	555.715	

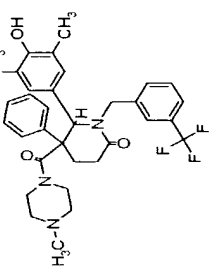
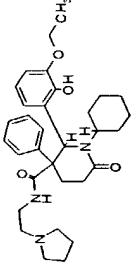
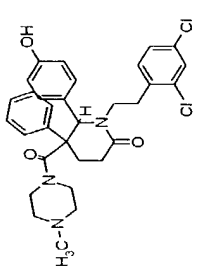
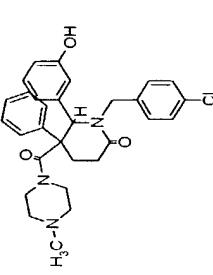
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Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc.mg/ml	LionID			
9100	2213	1	000727356	9100-031	E 08	0 271	Spy4H	61.41	0 1776	0.1776	TR0910002213		C <sub>37</sub> H <sub>38</sub> F N <sub>3</sub> O <sub>3</sub>	591.723
9100	2738	1	000727881	9100-039	B 04	0 398	Spy4H	61.32	0 1776	0.1776	TR0910002738		C <sub>31</sub> H <sub>25</sub> Cl N <sub>2</sub> O <sub>4</sub> S	561.099
9100	979	1	000726362	9100-013	C 04	0 245	Spy4H	61.31	0 1776	0.1776	TR0910000979		C <sub>30</sub> H <sub>39</sub> Br N <sub>4</sub> O <sub>4</sub>	599.566
9100	1019	1	000726402	9100-013	C 09	0 239	Spy4H	61.31	0 1776	0.1776	TR0910001019		C <sub>25</sub> H <sub>41</sub> N <sub>3</sub> O <sub>3</sub>	479.661

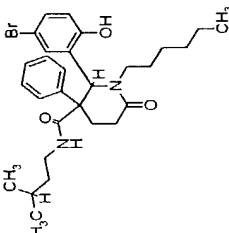
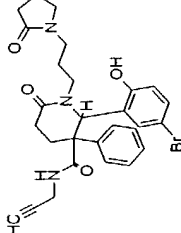
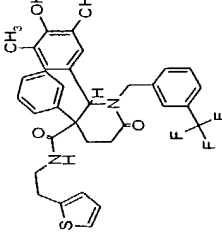
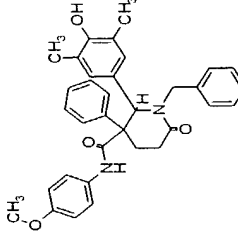


Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?						
9100	1002	1	000726385	9100-013	B 07	0.24	61.04	Spy4H	0.1776	0.1776		TR0910001002						C <sub>30</sub> H <sub>41</sub> N <sub>3</sub> O <sub>3</sub>	491.672
9100	1004	1	000726387	9100-013	D 07	0.242	61.04	Spy4H	0.1776	0.1776		TR0910001004						C <sub>28</sub> H <sub>36</sub> N <sub>4</sub> O <sub>3</sub>	488.628
9100	621	1	000726004	9100-008	E 09	0.29	61.03	Spy4H	0.1776	0.1776		TR0910000621						C <sub>28</sub> H <sub>34</sub> N <sub>2</sub> O <sub>3</sub>	422.566
9100	2221	1	000727364	9100-031	E 09	0.251	60.87	Spy4H	0.1776	0.1776		TR0910002221						C <sub>35</sub> H <sub>43</sub> N <sub>3</sub> O <sub>3</sub>	553.743

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID			
9100	689	1	000726072	9100-009	A 08	0.249	60.79	Spy4H	0.1776	TR0910000689		C <sub>33</sub> H <sub>36</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	579.659
9100	2322	1	000727465	9100-033	B 02	0.255	60.75	Spy4H	0.1776	TR0910002322		C <sub>32</sub> H <sub>43</sub> N <sub>3</sub> O <sub>4</sub>	533.709
9100	2969	1	000728112	9100-042	A 03	0.328	60.74	Spy4H	0.1776	TR0910002969		C <sub>31</sub> H <sub>33</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	566.526
9100	849	1	000726232	9100-011	A 08	0.295	60.55	Spy4H	0.1776	TR0910000849		C <sub>30</sub> H <sub>32</sub> Cl N <sub>3</sub> O <sub>3</sub>	518.054

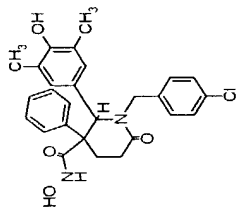
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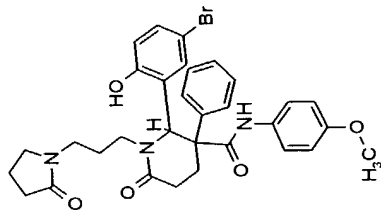
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc	mg/ml	LionID	#NAME?		
9100	2461	1	000727604	9100-035	E 09	0.402	60.32	Spy4H	0.1776		TR0910002461		C <sub>29</sub> H <sub>39</sub> Br N <sub>2</sub> O <sub>3</sub>	543.542
														
9100	990	1	000726373	9100-013	F 05	0.26	60.23	Spy4H	0.1776		TR0910000990	#NAME?	C <sub>28</sub> H <sub>30</sub> Br N <sub>3</sub> O <sub>4</sub>	552.466
														
9100	711	1	000726094	9100-009	G 10	0.388	60.12	Spy4H	0.1776		TR0910000711	#NAME?	C <sub>34</sub> H <sub>33</sub> F <sub>3</sub> N <sub>2</sub> O <sub>3</sub> S	606.706
														
9100	2436	1	000727579	9100-035	D 06	0.314	60.00	Spy4H	0.1776		TR0910002436	#NAME?	C <sub>34</sub> H <sub>34</sub> N <sub>2</sub> O <sub>4</sub>	534.653
														

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc(mg/ml)	LionID	#NAME?		Molecular Formula	Mass
9100	2339	1	000727482	9100-033	C 04	0.257	Spy4H	59.91	Assay	0.1776	TR0910002339		<chem>CCN(C)CCNC(=O)C1CC2C(C1)C(O)C(=O)C2C3C(C)C(CO)C3</chem>	C <sub>31</sub> H <sub>43</sub> N <sub>3</sub> O <sub>4</sub>	521.698
9100	572	1	000725955	9100-008	D 03	0.338	Spy4H	59.88	Assay	0.1776	TR0910000572			C <sub>29</sub> H <sub>31</sub> F N <sub>2</sub> O <sub>3</sub>	474.573
9100	1061	1	000726444	9100-014	E 04	0.403	Spy4H	59.84	Assay	0.1776	TR0910001061			C <sub>28</sub> H <sub>36</sub> N <sub>2</sub> O <sub>3</sub>	448.603
9100	857	1	000726240	9100-011	A 09	0.265	Spy4H	59.74	Assay	0.1776	TR0910000857			C <sub>27</sub> H <sub>27</sub> Cl N <sub>2</sub> O <sub>4</sub>	478.973
9100	861	1	000726244	9100-011	E 09	0.427	Spy4H	59.74	Assay	0.1776	TR0910000861			C <sub>30</sub> H <sub>33</sub> Cl N <sub>2</sub> O <sub>3</sub>	505.055

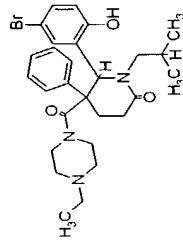
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>27</sub> H <sub>27</sub> Cl N <sub>2</sub> O <sub>4</sub>	478.973
9100	2637	1	000727780	9100-037	E 11	0.35	59.73	Spy4H	0.1776	TR0910002637			



9100	996	1	000726379	9100-013	D 06	0.279	59.69	Spy4H	0.1776	TR0910000996		C <sub>32</sub> H <sub>34</sub> Br N <sub>3</sub> O <sub>5</sub>	620.541
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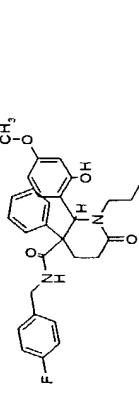

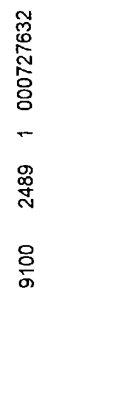


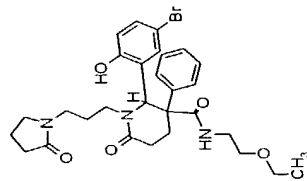
9100	1700	1	000726843	9100-023	D 04	0.316	59.50	Spy4H	0.1776	TR0910001700		C <sub>28</sub> H <sub>38</sub> Br N <sub>3</sub> O <sub>3</sub>	542.514
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478.973 : 620.541 : 542.514



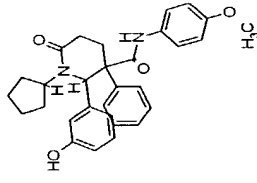
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?	Chemical Structure	C <sub>31</sub> H <sub>35</sub> F N <sub>2</sub> O <sub>5</sub>	534.625
9100	813	1	000726196	9100-011	E 03	0.38	59.47	Spy4H	0.1776	0.1776	TR0910000813				
9100	2489	1	000727632	9100-036	A 03	0.361	59.45	Spy4H	0.1776	0.1776	TR0910002489			C <sub>33</sub> H <sub>37</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	594.579
9100	988	1	000726371	9100-013	D 05	0.247	59.42	Spy4H	0.1776	0.1776	TR0910000988			C <sub>25</sub> H <sub>36</sub> Br N <sub>3</sub> O <sub>5</sub>	586.523

[illegible]

Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	IonID
9100	3236	1	000728379	9100-045	D 06	0 304	59 42	Spy4H	0 1776	TR0910003236	#NAME?

C<sub>30</sub> H<sub>32</sub> N<sub>2</sub> O<sub>4</sub>

484.593



C<sub>33</sub> H<sub>38</sub> N<sub>2</sub> O<sub>4</sub>

526.673

#NAME?

TR0910002438

Spy4H

59 36

0 285

F 06

9100-035

0 1776

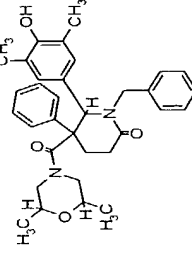
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Spy4H

59 36

0 285

F 06



C<sub>27</sub> H<sub>34</sub> N<sub>2</sub> O<sub>3</sub>

434.577

#NAME?

TR0910001115

Spy4H

59 28

0 262

C 11

9100-014

0 1776

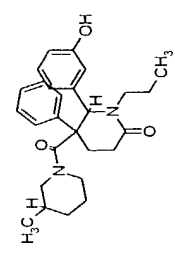
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Spy4H

59 28

0 262

C 11



C<sub>27</sub> H<sub>35</sub> Br N<sub>2</sub> O<sub>3</sub>

515.489

#NAME?

TR0910001701

Spy4H

59 24

0 512

E 04

9100-023

0 1776

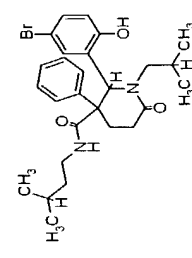
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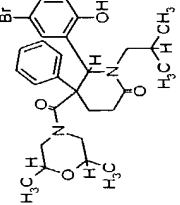
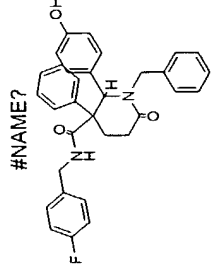
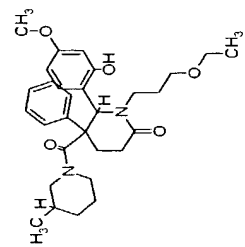
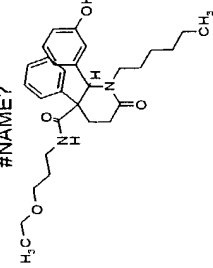
Spy4H

59 24

0 512

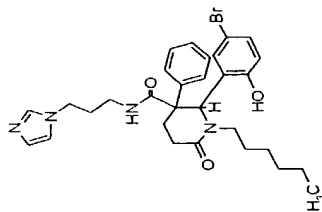
E 04



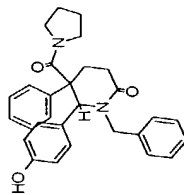
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>28</sub> H <sub>35</sub> Br N <sub>2</sub> O <sub>4</sub>	543 498
9100	1718	1	000726861	9100-023	F 06	0 364	59 24	Spy4H	0 1776	TR0910001718			
9100	1733	1	000726876	9100-023	E 08	0 331	59 24	Spy4H	0 1776	TR0910001733		C <sub>32</sub> H <sub>29</sub> F N <sub>2</sub> O <sub>3</sub>	508 59
9100	835	1	000726218	9100-011	C 06	0 321	59 20	Spy4H	0 1776	TR0910000835		C <sub>30</sub> H <sub>40</sub> N <sub>2</sub> O <sub>5</sub>	508 655
9100	1022	1	000726405	9100-013	F 09	0 261	59 15	Spy4H	0 1776	TR0910001022		C <sub>29</sub> H <sub>40</sub> N <sub>2</sub> O <sub>4</sub>	480 645

1718 1733 835 1022

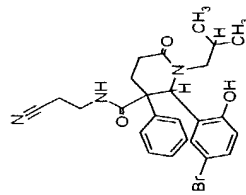
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc	mg/ml	LionID	#NAME?	C <sub>30</sub> H <sub>37</sub> Br N <sub>4</sub> O <sub>3</sub>	581.551
9100	2454	1	000727597	9100-035	F 08	0.283	59.04	Spy4H	0.1776		TR0910002454			



9100	1723	1	000726866	9100-023	C 07	0.289	58.97	Spy4H	0.1776		TR0910001723	#NAME?	C <sub>29</sub> H <sub>30</sub> N <sub>2</sub> O <sub>3</sub>	454.567
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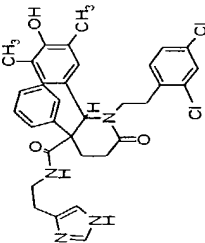
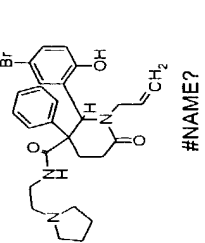
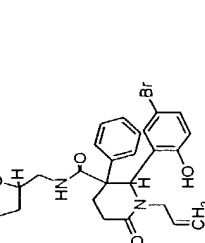
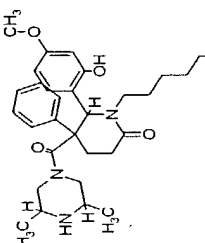


9100	1714	1	000726857	9100-023	B 05	0.335	58.70	Spy4H	0.1776		TR0910001714	#NAME?	C <sub>25</sub> H <sub>28</sub> Br N <sub>3</sub> O <sub>3</sub>	498.418
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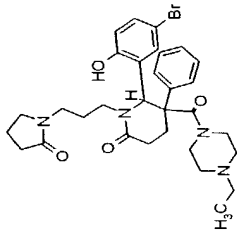
40524522 # 000000



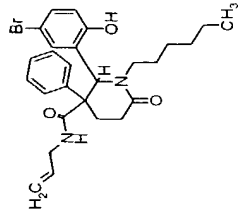
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	C <sub>33</sub> H <sub>34</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>3</sub>	605.563
9100	2484	1	000727627	9100-036	D 02	0 319	58 38	Spy4H	0 1776	TR0910002484					
9100	202	1	000725585	9100-003	B 07	0 243	58 34	Spy4H	0 1776	TR0910000202					
9100	210	1	000725593	9100-003	B 08	0 331	58 34	Spy4H	0 1776	TR0910000210					
9100	3029	1	000728172	9100-042	E 10	0 279	58 29	Spy4H	0 1776	TR0910003029					



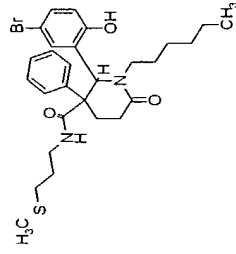
Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	$C_{21}H_{33}BrN_4O_4$	611.577
9100	980	1	000726363	9100-013	D 04	0.254	58.06	Spy4H	0.1776	TR0910000980			



9100	2446	1	000727589	9100-035	F 07	0.408	57.76	Spy4H	0.1776	TR0910002446	#NAME?	$C_{27}H_{33}BrN_2O_3$	513.473
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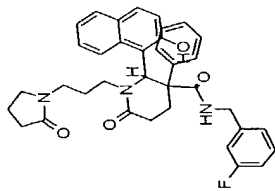


9100	2465	1	000727608	9100-035	A 10	0.25	57.76	Spy4H	0.1776	TR0910002465	#NAME?	$C_{28}H_{37}BrN_2O_3S$	561.581
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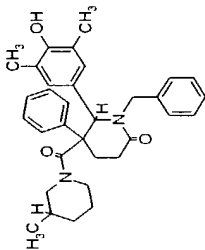




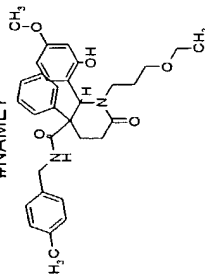
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>36</sub> H <sub>36</sub> F N <sub>3</sub> O <sub>4</sub>	593.695
9100	3732	1	000728875	9100-051	D 08	0 312	57.63	Spy4H	0.1776	TR0910003732			



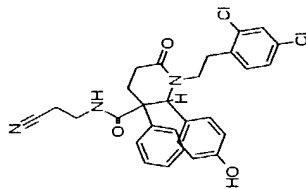
9100	2435	1	000727578	9100-035	C 06	0 395	57.43	Spy4H	0.1776	TR0910002435	#NAME?	C <sub>33</sub> H <sub>38</sub> N <sub>2</sub> O <sub>3</sub>	510.674
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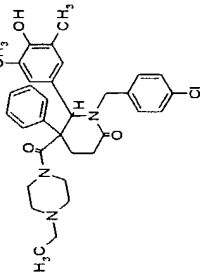
9100	811	1	000726194	9100-011	C 03	0 377	57.30	Spy4H	0.1776	TR0910000811	#NAME?	C <sub>32</sub> H <sub>38</sub> N <sub>2</sub> O <sub>5</sub>	530.661
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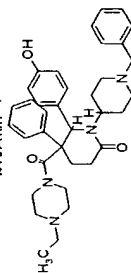
Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>29</sub> H <sub>27</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	536.456
9100	2994	1	000728137	9100-042	B 06	0.413	57.20	Spy4H	0.1776	TR0910002994			



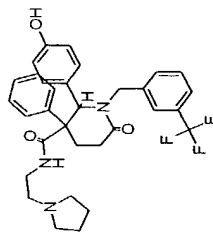
9100	2620	1	000727763	9100-037	D 09	0.268	57.14	Spy4H	0.1776	TR0910002620	#NAME?	C <sub>33</sub> H <sub>38</sub> Cl N <sub>3</sub> O <sub>3</sub>	560.134
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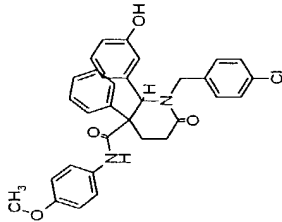
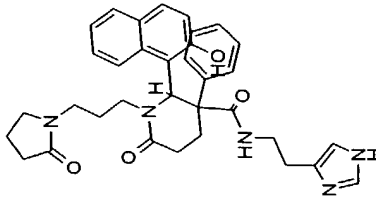
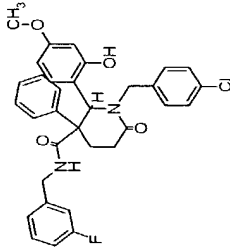


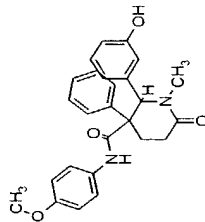
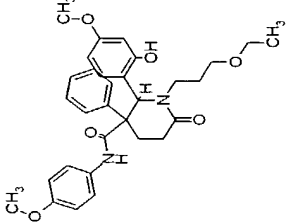
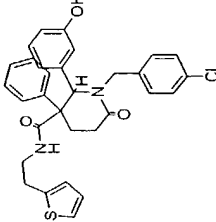
9100	2580	1	000727723	9100-037	D 04	0.243	56.86	Spy4H	0.1776	TR0910002580	#NAME?	C <sub>36</sub> H <sub>44</sub> N <sub>4</sub> O <sub>3</sub>	580.769
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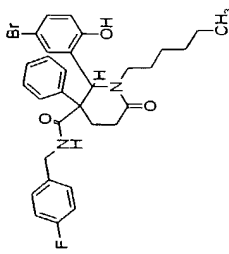
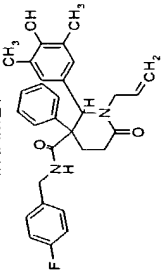
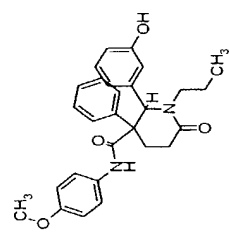
9100	4082	1	000729225	9100-057	B 02	0.248	56.80	Spy4H	0.1776	TR0910004082	#NAME?	C <sub>32</sub> H <sub>34</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	565.633
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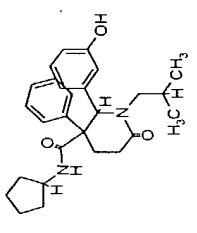
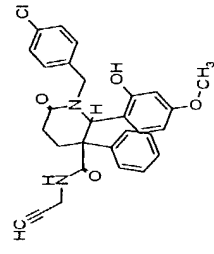
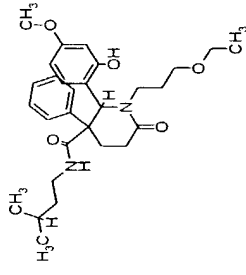
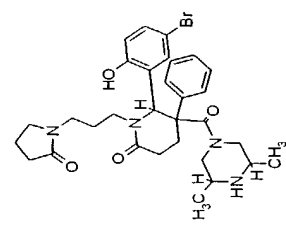
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>32</sub> H <sub>29</sub> Cl N <sub>2</sub> O <sub>4</sub>	541.044
9100	876	1	000726259	9100-011	D 11	0.432	56.76	Spy4H	0.1776	TR0910000876				
9100	3724	1	000728867	9100-051	D 07	0.252	56.72	Spy4H	0.1776	TR0910003724			C <sub>34</sub> H <sub>37</sub> N <sub>5</sub> O <sub>4</sub>	579.697
9100	2732	1	000727875	9100-039	D 03	0.457	56.68	Spy4H	0.1776	TR0910002732			C <sub>33</sub> H <sub>30</sub> Cl F N <sub>2</sub> O <sub>4</sub>	573.061

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?	$C_{26}H_{26}N_2O_4$	430.501
9100	196	1	000725579	9100-003	D 06	0.252	Spy4H	56.51	0.1776	0.1776	TR0910000196			
9100	836	1	000726219	9100-011	D 06	0.304	Spy4H	56.49	0.1776	0.1776	TR0910000836		$C_{31}H_{36}N_2O_5$	532.633
9100	871	1	000726254	9100-011	G 10	0.336	Spy4H	56.49	0.1776	0.1776	TR0910000871		$C_{31}H_{26}ClN_2O_3S$	545.1

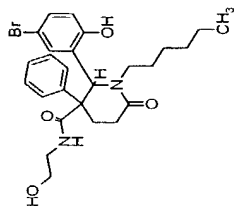
100943552, 0203202

Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>31</sub> H <sub>34</sub> Br F N <sub>2</sub> O <sub>3</sub>	581.523
9100	2453	1	000727596	9100-035	E 08	0.43	56.47	Spy4H	0.1776	TR0910002453			
9100	1053	1	000726436	9100-014	E 03	0.478	56.44	Spy4H	0.1776	TR0910001053		486.584	
9100	1116	1	000726499	9100-014	D 11	0.265	56.44	Spy4H	0.1776	TR0910001116		458.555	
9100	997	1	000726380	9100-013	E 06	0.254	56.44	Spy4H	0.1776	TR0910000997		530.416	

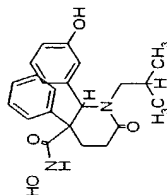
93

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc.mg/ml	LionID	#NAME?	C <sub>27</sub> H <sub>34</sub> N <sub>2</sub> O <sub>3</sub>	434.577
9100	565	1	000725948	9100-008	E 02	0 304	Spy4H	56.40	0 1776	TR0910000565				
9100	2750	1	000727893	9100-039	F 05	0 457	Spy4H	56.39	0 1776	TR0910002750			C <sub>28</sub> H <sub>27</sub> Cl N <sub>2</sub> O <sub>4</sub>	502.995
9100	821	1	000726204	9100-011	E 04	0 322	Spy4H	56.22	0 1776	TR0910000821			C <sub>29</sub> H <sub>40</sub> N <sub>2</sub> O <sub>5</sub>	496.644
9100	989	1	000726372	9100-013	E 05	0 257	Spy4H	56.17	0 1776	TR0910000989			C <sub>31</sub> H <sub>38</sub> Br N <sub>4</sub> O <sub>4</sub>	611.577

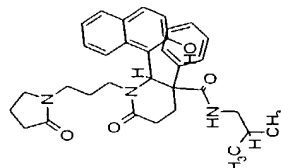
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>26</sub> H <sub>33</sub> Br N <sub>2</sub> O <sub>4</sub>	517.461
9100	2457	1	000727600	9100-035	A 09	0.275	56.15	Spy4H	0.1776	TR0910002457			



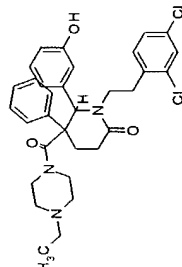
9100	597	1	000725980	9100-008	E 06	0.25	56.11	Spy4H	0.1776	TR0910000597	#NAME?	C <sub>22</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>	382.457
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9100	3746	1	000728889	9100-051	B 10	0.268	56.11	Spy4H	0.1776	TR0910003746	#NAME?	C <sub>33</sub> H <sub>39</sub> N <sub>3</sub> O <sub>4</sub>	541.688
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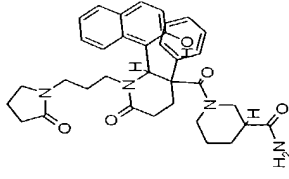
9100	660	1	000726043	9100-009	D 04	0.433	56.07	Spy4H	0.1776	TR0910000660	#NAME?	C <sub>32</sub> H <sub>35</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	580.552
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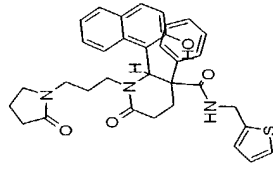
[illegible]



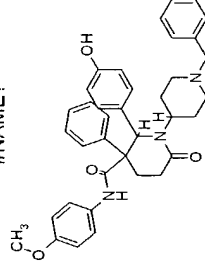
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	C <sub>35</sub> H <sub>40</sub> N <sub>4</sub> O <sub>5</sub>	596 724
9100	3721	1	000728864	9100-051	A 07	0.298	55.80	Spy4H	0.1776	TR0910003721					



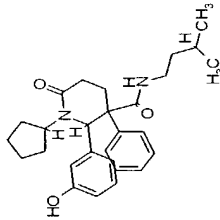
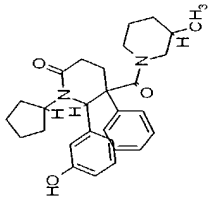
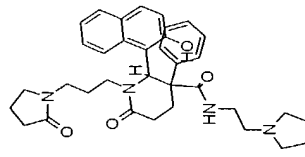
9100	3738	1	000728881	9100-051	B 09	0.275	55.80	Spy4H	0.1776	TR0910003738				C <sub>34</sub> H <sub>35</sub> N <sub>3</sub> O <sub>4</sub> S	581 734
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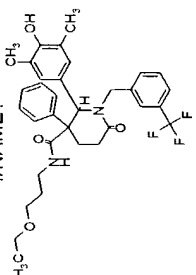
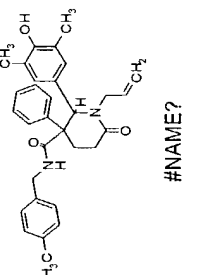
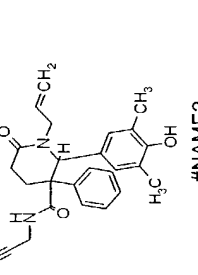
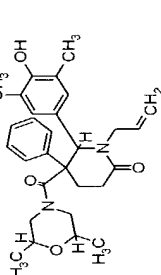
9100	2596	1	000727739	9100-037	D 06	0.263	55.71	Spy4H	0.1776	TR0910002596				C <sub>37</sub> H <sub>39</sub> N <sub>3</sub> O <sub>4</sub>	589.732
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10091593 # 000300

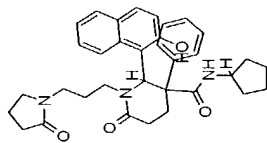
Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>28</sub> H <sub>36</sub> N <sub>2</sub> O <sub>3</sub>	448 603
9100	3221	1	000728364	9100-045	E 04	0.375	55.66	Spy4H	0.1776	TR0910003221				
9100	3235	1	000728378	9100-045	C 06	0.352	55.66	Spy4H	0.1776	TR0910003235			460 614	
9100	3722	1	000728865	9100-051	B 07	0.26	55.50	Spy4H	0.1776	TR0910003722			582 741	

400945997 #0009997

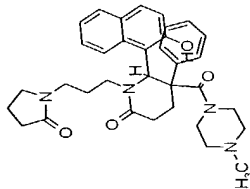
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc mg/ml	LionID	#NAME?			
9100	702	1	000726085	9100-009	F 09	0.29	55.40	Spy4H	0.1776	TR0910000702	TR0910000702		C <sub>33</sub> H <sub>37</sub> F <sub>3</sub> N <sub>2</sub> O <sub>4</sub>	582.659	
9100	1051	1	000726434	9100-014	C 03	0.422	55.31	Spy4H	0.1776	TR0910001051	TR0910001051		C <sub>31</sub> H <sub>34</sub> N <sub>2</sub> O <sub>3</sub>	482.621	
9100	1070	1	000726453	9100-014	F 05	0.255	55.31	Spy4H	0.1776	TR0910001070	TR0910001070		C <sub>26</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>	416.518	
9100	1078	1	000726461	9100-014	F 06	0.255	55.31	Spy4H	0.1776	TR0910001078	TR0910001078		C <sub>29</sub> H <sub>36</sub> N <sub>2</sub> O <sub>4</sub>	476.613	

409944492 # 00000000

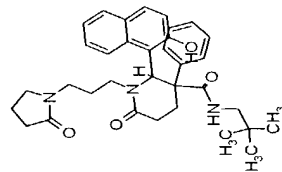
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>34</sub> H <sub>35</sub> N <sub>3</sub> O <sub>4</sub>	553.699
9100	3725	1	000728868	9100-051	E 07	0.264	55.19	Spy4H	0.1776	TR0910003725			

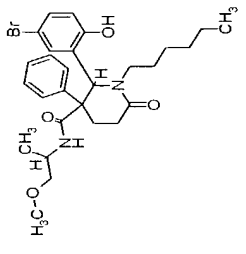
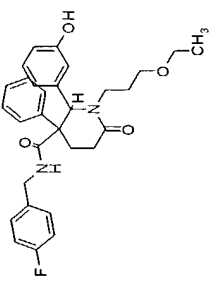
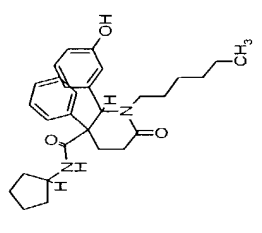
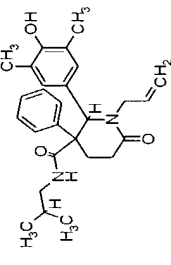


9100	3729	1	000728872	9100-051	A 08	0.301	55.19	Spy4H	0.1776	TR0910003729	#NAME?	C <sub>34</sub> H <sub>40</sub> N <sub>4</sub> O <sub>4</sub>	568.714
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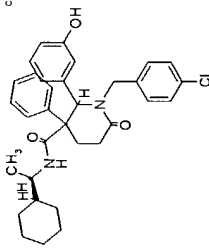
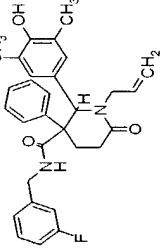
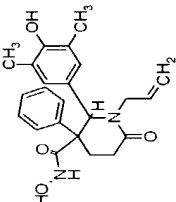
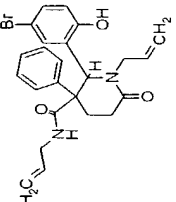
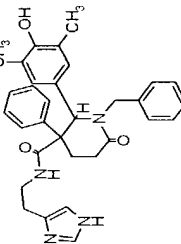


9100	3744	1	000728887	9100-051	H 09	0.268	55.19	Spy4H	0.1776	TR0910003744	#NAME?	C <sub>34</sub> H <sub>41</sub> N <sub>3</sub> O <sub>4</sub>	555.715
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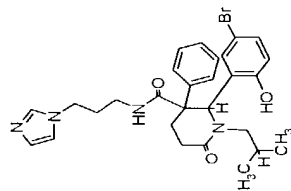
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>28</sub> H <sub>37</sub> Br N <sub>2</sub> O <sub>4</sub>	545.514
9100	2473	1	000727616	9100-035	A 11	0.334	55.19	Spy4H	0.1776	TR0910002473			
9100	1973	1	000727116	9100-028	E 08	0.28	55.14	Spy4H	0.1776	TR0910001973		C <sub>30</sub> H <sub>33</sub> F N <sub>2</sub> O <sub>4</sub>	504.599
9100	1005	1	000726388	9100-013	E 07	0.445	55.08	Spy4H	0.1776	TR0910001005		C <sub>29</sub> H <sub>38</sub> N <sub>2</sub> O <sub>3</sub>	462.63
9100	1066	1	000726449	9100-014	B 05	0.305	55.03	Spy4H	0.1776	TR0910001066		C <sub>27</sub> H <sub>34</sub> N <sub>2</sub> O <sub>3</sub>	434.577

10034305 : 000305

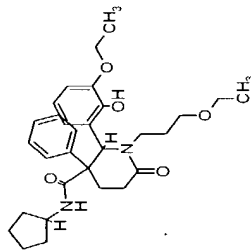
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?		Formula	Mass
9100	863	1	000726246	9100-011	G 09	0.487	54.87	Spy4H	0.1776	TR0910000863	545.119	C <sub>33</sub> H <sub>37</sub> Cl N <sub>2</sub> O <sub>3</sub>				
9100	1052	1	000726435	9100-014	D 03	0.419	54.75	Spy4H	0.1776	TR0910001052	486.584	C <sub>30</sub> H <sub>31</sub> F N <sub>2</sub> O <sub>3</sub>				
9100	1077	1	000726460	9100-014	E 06	0.257	54.75	Spy4H	0.1776	TR0910001077	394.468	C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub>				
9100	206	1	000725589	9100-003	F 07	0.305	54.68	Spy4H	0.1776	TR0910000206	469.376	C <sub>24</sub> H <sub>25</sub> Br N <sub>2</sub> O <sub>3</sub>				
9100	2404	1	000727547	9100-035	D 02	0.242	54.55	Spy4H	0.1776	TR0910002404	522.646	C <sub>32</sub> H <sub>34</sub> N <sub>4</sub> O <sub>3</sub>				



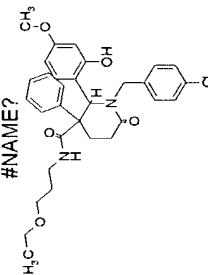
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	C <sub>28</sub> H <sub>33</sub> Br N <sub>4</sub> O <sub>3</sub>	553.498
9100	1694	1	000726837	9100-023	F 03	0.304	54 15	Spy4H	0.1776	TR0910001694					



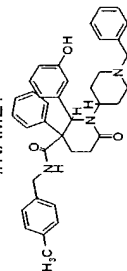
9100	2525	1	000727668	9100-036	E 07	0.325	54 11	Spy4H	0.1776	TR0910002525				C <sub>30</sub> H <sub>40</sub> N <sub>2</sub> O <sub>5</sub>	508.655
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9100	2742	1	000727885	9100-039	F 04	0.4	54.06	Spy4H	0.1776	TR0910002742				C <sub>31</sub> H <sub>35</sub> Cl N <sub>2</sub> O <sub>5</sub>	551.08
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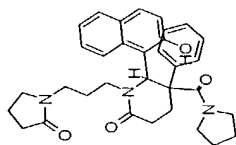


9100	2211	1	000727354	9100-031	C 08	0.323	54 05	Spy4H	0.1776	TR0910002211				C <sub>38</sub> H <sub>41</sub> N <sub>3</sub> O <sub>3</sub>	587.76
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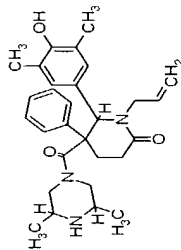




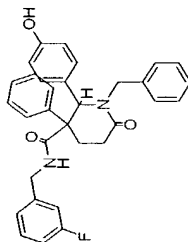
Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>33</sub> H <sub>37</sub> N <sub>3</sub> O <sub>4</sub>	539.672
9100	3723	1	000728866	9100-051	C 07	0.28	53.97	Spy4H	0.1776	TR0910003723			



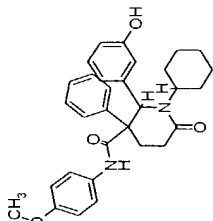
9100	1069	1	000726452	9100-014	E 05	0.259	53.90	Spy4H	0.1776	TR0910001069	#NAME?	C <sub>29</sub> H <sub>37</sub> N <sub>3</sub> O <sub>3</sub>	475.629
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9100	1732	1	000726875	9100-023	D 08	0.333	53.88	Spy4H	0.1776	TR0910001732	#NAME?	C <sub>32</sub> H <sub>25</sub> F N <sub>2</sub> O <sub>3</sub>	508.59
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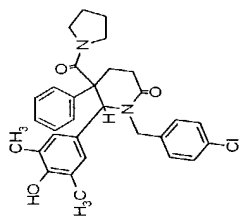


9100	4396	1	000729539	9100-060	D 11	0.347	53.87	Spy4H	0.1776	TR0910004396	#NAME?	C <sub>31</sub> H <sub>34</sub> N <sub>2</sub> O <sub>4</sub>	498.62
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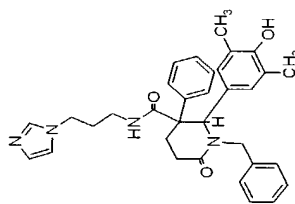




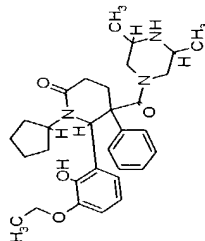
Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>31</sub> H <sub>33</sub> Cl N <sub>2</sub> O <sub>3</sub>	517.066
9100	2603	1	000727746	9100-037	C 07	0.467	53.70	Spy4H	0.1776	TR0910002603			



9100	2414	1	000727557	9100-035	F 03	0.258	53.59	Spy4H	0.1776	TR0910002414	#NAME?	C <sub>33</sub> H <sub>36</sub> N <sub>4</sub> O <sub>3</sub>	536.672
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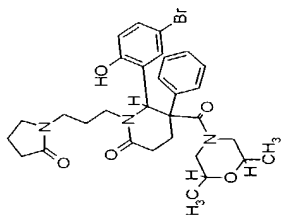


9100	1949	1	000727092	9100-028	E 05	0.281	53.49	Spy4H	0.1776	TR0910001949	#NAME?	C <sub>31</sub> H <sub>41</sub> N <sub>3</sub> O <sub>4</sub>	519.682
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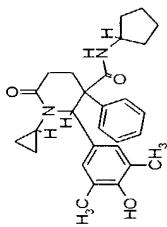


10091505 # 060500

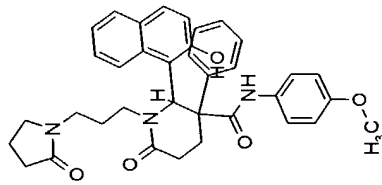
Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID
9100	998	1	000726381	9100-013	F 06	0.276	53.46	Spy4H	0.1776	TR0910000998	612.561	C <sub>31</sub> H <sub>35</sub> Br N <sub>3</sub> O <sub>5</sub>



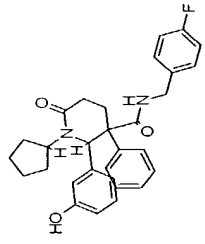
9100	765	1	000726148	9100-010	E 07	0.252	53.41	Spy4H	0.1776	TR0910000765	446.588	C <sub>28</sub> H <sub>34</sub> N <sub>2</sub> O <sub>3</sub>
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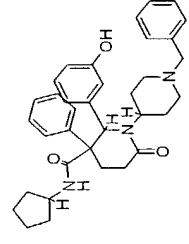
9100	3756	1	000728899	9100-051	D 11	0.288	53.36	Spy4H	0.1776	TR0910003756	591.704	C <sub>36</sub> H <sub>37</sub> N <sub>3</sub> O <sub>5</sub>
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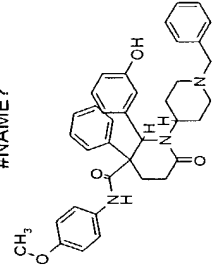
Library	Cmpd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc.mg/ml	LionID	#NAME?	C <sub>30</sub> H <sub>31</sub> F N <sub>2</sub> O <sub>3</sub>	486 584
9100	3213	1	000728356	9100-045	E-03	0.422	53.24	Spy4H	0 1776	TR0910003213				



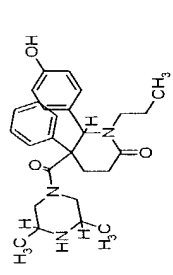
9100	2205	1	000727348	9100-031	E-07	0.27	53.24	Spy4H	0 1776	TR0910002205			C <sub>35</sub> H <sub>41</sub> N <sub>3</sub> O <sub>3</sub>	551.727
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9100	2236	1	000727379	9100-031	D-11	0.276	53.24	Spy4H	0 1776	TR0910002236			C <sub>37</sub> H <sub>39</sub> N <sub>3</sub> O <sub>4</sub>	589.732
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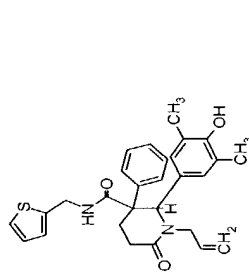


9100	629	1	000726012	9100-008	E-10	0.258	53.22	Spy4H	0 1776	TR0910000629			C <sub>27</sub> H <sub>35</sub> N <sub>3</sub> O <sub>3</sub>	449 591
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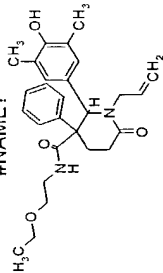


486 584 551 727 589 732 449 591

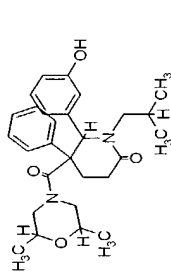
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	Lion ID	#NAME?	C <sub>28</sub> H <sub>30</sub> N <sub>2</sub> O <sub>3</sub> S	474.622
9100	1058	1	000726441	9100-014	B 04	0.351	53.05	Spy4H	0.1776	TR0910001058			



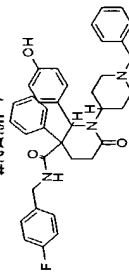
9100	1068	1	000726451	9100-014	D 05	0.261	53.05	Spy4H	0.1776	TR0910001068	#NAME?	C <sub>27</sub> H <sub>34</sub> N <sub>2</sub> O <sub>4</sub>	450.576
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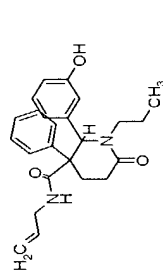
9100	598	1	000725981	9100-008	F 06	0.264	52.93	Spy4H	0.1776	TR0910000598	#NAME?	C <sub>28</sub> H <sub>36</sub> N <sub>2</sub> O <sub>4</sub>	464.602
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9100	2573	1	000727716	9100-037	E 03	0.287	52.84	Spy4H	0.1776	TR0910002573	#NAME?	C <sub>37</sub> H <sub>38</sub> F N <sub>3</sub> O <sub>3</sub>	591.723
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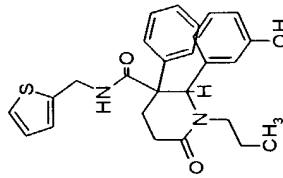


9100	1086	1	000726469	9100-014	F 07	0.263	52.76	Spy4H	0.1776	TR0910001086	#NAME?	C <sub>24</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>	392.496
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Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID
9100	1098	1	000726481	9100-014	B 09	0.298	52.76	Spy4H	0.1776	TR0910001098		

C<sub>26</sub> H<sub>28</sub> N<sub>2</sub> O<sub>3</sub> S 448.584



C<sub>37</sub> H<sub>45</sub> N<sub>3</sub> O<sub>4</sub> 595.779

#NAME?

TR0910003743

0.1776

Spy4H

52.75

0.347

G 09

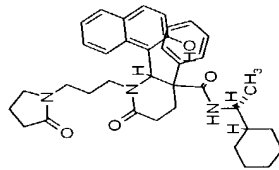
9100-051

000728886

3743

9100

Chem



C<sub>31</sub> H<sub>35</sub> F N<sub>2</sub> O<sub>5</sub> 534.625

#NAME?

TR0910000812

0.1776

Spy4H

52.70

0.339

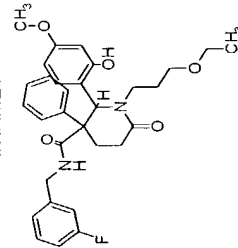
D 03

9100-011

000726195

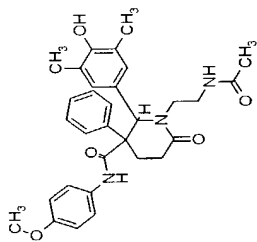
812

9100

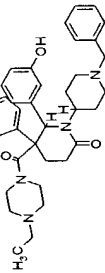


Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID
9100	2196	1	000727339	9100-031	D 06	0.271	52.69	Spy4H	0.1776	TR0910002196		

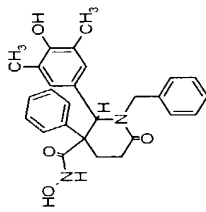
#NAME? C<sub>31</sub> H<sub>35</sub> N<sub>3</sub> O<sub>5</sub> 529 633



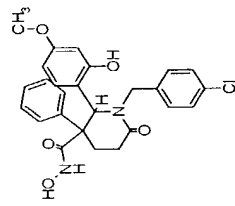
#NAME? C<sub>36</sub> H<sub>44</sub> N<sub>4</sub> O<sub>3</sub> 580 769



#NAME? C<sub>27</sub> H<sub>28</sub> N<sub>2</sub> O<sub>4</sub> 444 528



#NAME? C<sub>26</sub> H<sub>25</sub> Cl N<sub>2</sub> O<sub>5</sub> 480 945



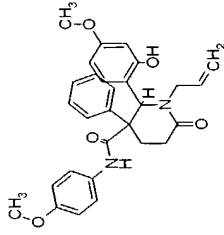


Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID
9100	2396	1	000727539	9100-033	D 11	0.334	52.60	Spv4H	0.1776	TR0910002396

C<sub>29</sub> H<sub>30</sub> N<sub>2</sub> O<sub>5</sub>

#NAME?

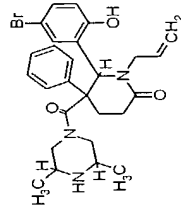
486.565



C<sub>27</sub> H<sub>32</sub> Br N<sub>3</sub> O<sub>3</sub>

#NAME?

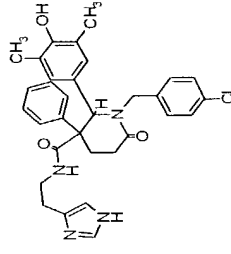
526.472



C<sub>32</sub> H<sub>33</sub> Cl N<sub>4</sub> O<sub>3</sub>

#NAME?

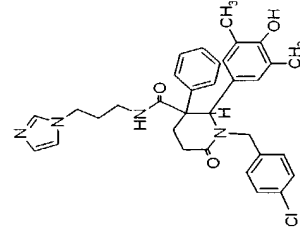
557.091

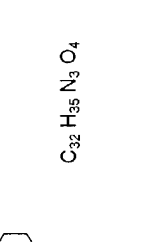
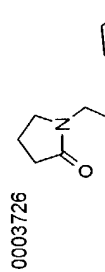
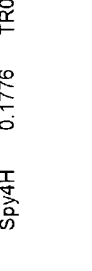


C<sub>33</sub> H<sub>35</sub> Cl N<sub>4</sub> O<sub>3</sub>

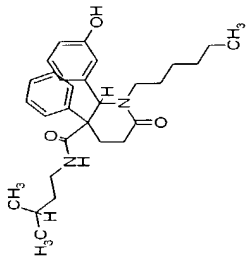
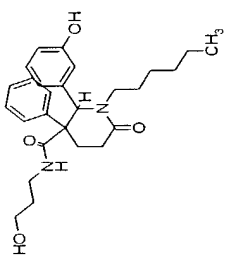
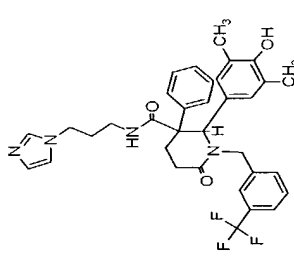
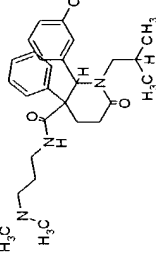
#NAME?

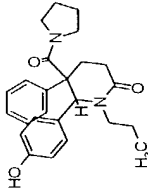
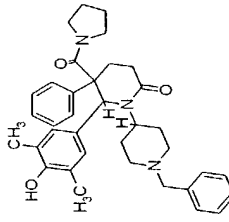
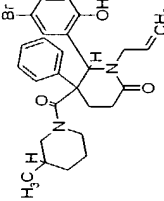
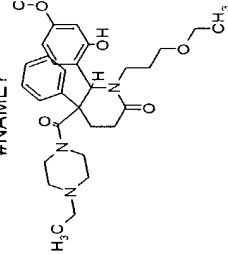
571.117



Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc.mg/ml	LionID	#NAME?	Chemical Structure	Formula	Mass
9100	3701	1	000728844	9100-051	E 04	0.418	52.44	Spy4H	0.1776	TR0910003701			C <sub>31</sub> H <sub>42</sub> N <sub>2</sub> O <sub>3</sub>	490.684
9100	3726	1	000728869	9100-051	F 07	0.275	52.44	Spy4H	0.1776	TR0910003726			C <sub>32</sub> H <sub>35</sub> N <sub>3</sub> O <sub>4</sub>	525.646
9100	3755	1	000728898	9100-051	C 11	0.294	52.44	Spy4H	0.1776	TR0910003755			C <sub>35</sub> H <sub>41</sub> N <sub>3</sub> O <sub>4</sub>	567.726

[illegible]

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	<chem>C29H40N2O3</chem>	464.646
9100	1021	1	000726404	9100-013	E 09	0.399	52.37	Spy4H	0.1776	TR0910001021			
9100	1027	1	000726410	9100-013	C 10	0.28	52.37	Spy4H	0.1776	TR0910001027		452.591	
9100	694	1	000726077	9100-009	F 08	0.285	52.36	Spy4H	0.1776	TR0910000694		604.669	
9100	579	1	000725962	9100-008	C 04	0.261	52.35	Spy4H	0.1776	TR0910000579		451.607	

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?			
9100	603	1	000725986	9100-008	C 07	0.269	52.35	Spy4H	0.1776	TR0910000603			$C_{25}H_{30}N_2O_3$	406.523
9100	4123	1	000729266	9100-057	C 07	0.289	52.30	Spy4H	0.1776	TR0910004123			$C_{36}H_{43}N_3O_3$	565.754
9100	235	1	000725618	9100-003	C 11	0.485	52.25	Spy4H	0.1776	TR0910000235			$C_{27}H_{31}BrN_2O_3$	511.457
9100	820	1	000726203	9100-011	D 04	0.272	52.16	Spy4H	0.1776	TR0910000820			$C_{30}H_{41}N_3O_5$	523.67

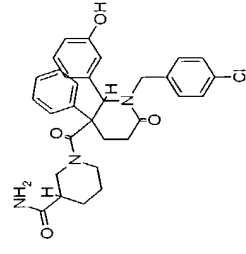
TR0910000603  
TR0910004123  
TR0910000235  
TR0910000820

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID
9100	841	1	000726224	9100-011	A 07	52.16	0.354	Spy4H	0.1776	TR0910000841

C<sub>31</sub> H<sub>32</sub> Cl N<sub>3</sub> O<sub>4</sub>

#NAME?

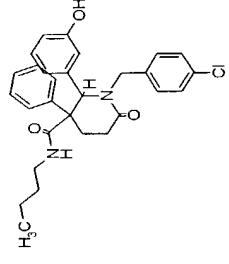
546.064



C<sub>29</sub> H<sub>31</sub> Cl N<sub>2</sub> O<sub>3</sub>

#NAME?

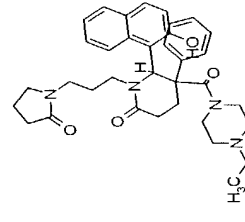
491.028



C<sub>35</sub> H<sub>42</sub> N<sub>4</sub> O<sub>4</sub>

#NAME?

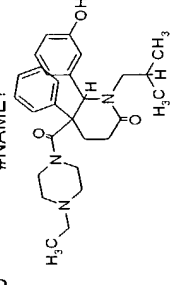
582.741

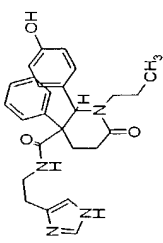
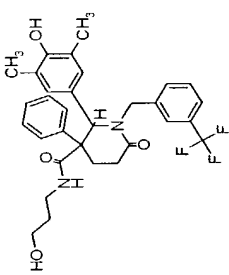
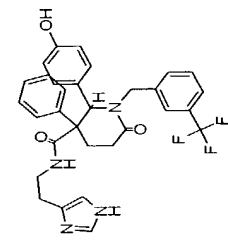
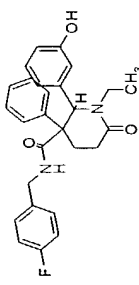


C<sub>28</sub> H<sub>37</sub> N<sub>3</sub> O<sub>3</sub>

#NAME?

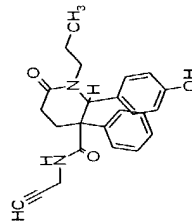
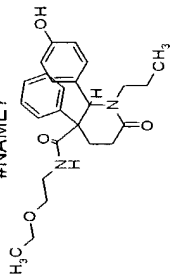
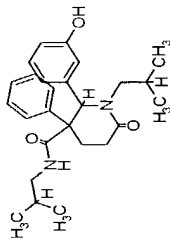
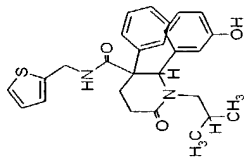
463.618



Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?			
9100	604	1	000725987	9100-008	D 07	0.261	Spy4H	52.06	0.1776	0.1776	TR0910000604	C <sub>26</sub> H <sub>30</sub> N <sub>4</sub> O <sub>3</sub>	446.548			
9100	707	1	000726090	9100-009	C 10	0.306	Spy4H	52.02	0.1776	0.1776	TR0910000707	C <sub>31</sub> H <sub>33</sub> F <sub>3</sub> N <sub>2</sub> O <sub>4</sub>	554.606			
9100	4084	1	000729227	9100-057	D 02	0.264	Spy4H	52.02	0.1776	0.1776	TR0910004084	C <sub>31</sub> H <sub>29</sub> F <sub>3</sub> N <sub>4</sub> O <sub>3</sub>	562.589			
9100	733	1	000726116	9100-010	E 03	0.253	Spy4H	51.92	0.1776	0.1776	TR0910000733	C <sub>27</sub> H <sub>27</sub> F N <sub>2</sub> O <sub>3</sub>	446.519			

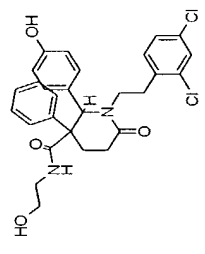
446.548 554.606 562.589 446.519

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc ng/ml	LionID	#NAME?	C <sub>27</sub> H <sub>30</sub> N <sub>2</sub> O <sub>3</sub> S	462.611
9100	578	1	000725961	9100-008	B 04	0.334	51.77	Spy4H	0.1776	TR0910000578				
9100	586	1	000725969	9100-008	B 05	0.301	51.77	Spy4H	0.1776	TR0910000586				
9100	628	1	000726011	9100-008	D 10	0.263	51.77	Spy4H	0.1776	TR0910000628				
9100	630	1	000726013	9100-008	F 10	0.264	51.77	Spy4H	0.1776	TR0910000630				



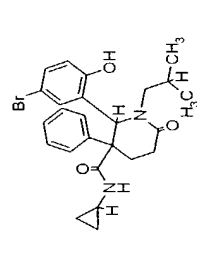
HOPELIFE-000000

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc.mg/ml	Lioid
9100	2977	1	000728120	9100-042	A 04	0.341	51.75	Spy4H	0.1776	TR0910002977



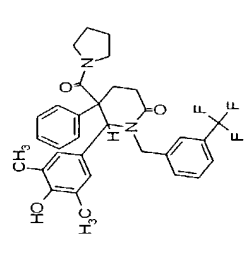
#NAME?  
C<sub>28</sub> H<sub>28</sub> Cl<sub>2</sub> N<sub>2</sub> O<sub>4</sub> 527.445

9100	1695	1	000726838	9100-023	G 03	0.442	51.74	Spy4H	0.1776	TR0910001695
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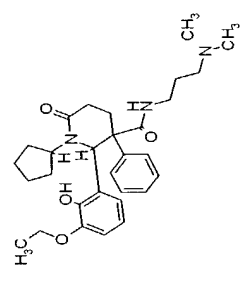
#NAME?  
C<sub>25</sub> H<sub>29</sub> Br N<sub>2</sub> O<sub>3</sub> 485.419

9100	683	1	000726066	9100-009	C 07	0.546	51.69	Spy4H	0.1776	TR0910000683
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#NAME?  
C<sub>32</sub> H<sub>33</sub> F<sub>3</sub> N<sub>2</sub> O<sub>3</sub> 550.618

9100	1939	1	000727082	9100-028	C 04	0.287	51.58	Spy4H	0.1776	TR0910001939
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#NAME?  
C<sub>30</sub> H<sub>41</sub> N<sub>3</sub> O<sub>4</sub> 507.671

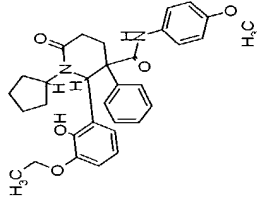


Library Compd Lot ExtReg Plate Well Raw Data Assay Result Assay Conc mg/ml LionID  
9100 1956 1 000727099 9100-028 D 06 0 29 51.58 Spy4H 0 1776 TR0910001956

C<sub>32</sub> H<sub>36</sub> N<sub>2</sub> O<sub>5</sub>

#NAME?

528.645

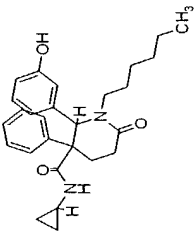


C<sub>27</sub> H<sub>34</sub> N<sub>2</sub> O<sub>3</sub>

#NAME?

434.577

9100 1015 1 000726398 9100-013 G 08 0 352 51.56 Spy4H 0 1776 TR0910001015

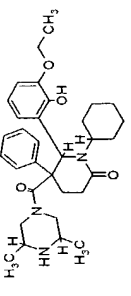


C<sub>32</sub> H<sub>43</sub> N<sub>3</sub> O<sub>4</sub>

#NAME?

533.709

9100 2349 1 000727492 9100-033 E 05 0 299 51.48 Spy4H 0 1776 TR0910002349

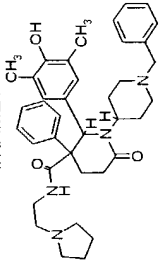


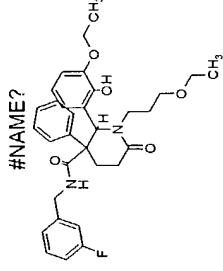
C<sub>38</sub> H<sub>48</sub> N<sub>4</sub> O<sub>3</sub>


#NAME?

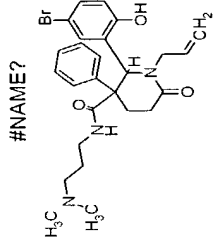
608.822

9100 4122 1 000729265 9100-057 B 07 0 273 51.46 Spy4H 0 1776 TR0910004122

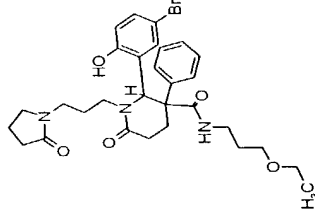


[illegible]

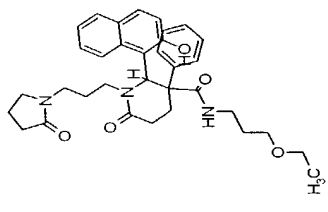
9100	219	1	000725602	9100-003	C 09	0.265	51.33	Spv4H	0.1776	TR0910000219	#NAME?	C <sub>28</sub> H <sub>32</sub> Br N <sub>3</sub> O <sub>3</sub>	514.461
													
9100	982	1	000726365	9100-013	F 04	0.28	51.29	Spv4H	0.1776	TR0910000982	#NAME?	C <sub>30</sub> H <sub>38</sub> Br N <sub>3</sub> O <sub>5</sub>	600.55



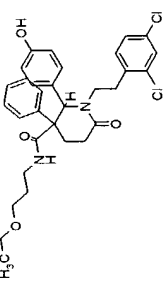
9100	982	1	000726365	9100-013	F 04	0 28	51.29	Spy4H	0.1776	TR0910000982	#NAME?	C <sub>30</sub> H <sub>38</sub> Br N <sub>3</sub> O <sub>5</sub>	600.55
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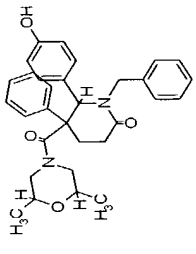
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc.mg/ml	LionID	#NAME?	C <sub>34</sub> H <sub>41</sub> N <sub>3</sub> O <sub>5</sub>	571.714
9100	3742	1	000728885	9100-051	F 09	0.276	Spy4H	51.22	0.1776	0.1776	TR0910003742			



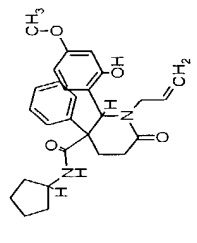
9100	2982	1	000728125	9100-042	F 04	0.438	Spy4H	51.21	0.1776	0.1776	TR0910002982	#NAME?	C <sub>31</sub> H <sub>34</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>	569 526
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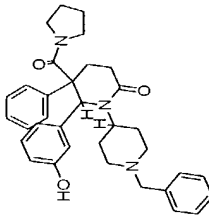


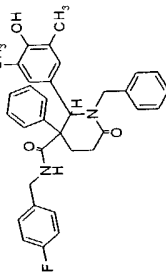
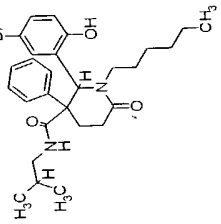
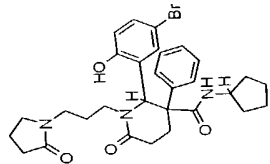
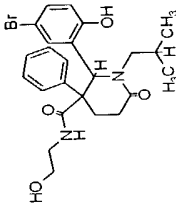
9100	1758	1	000726901	9100-023	F 11	0.298	Spy4H	51.20	0.1776	0.1776	TR0910001758	#NAME?	C <sub>31</sub> H <sub>34</sub> N <sub>2</sub> O <sub>4</sub>	498 62
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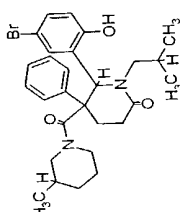
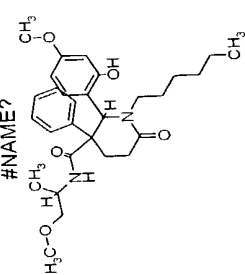
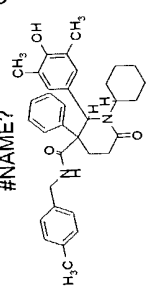
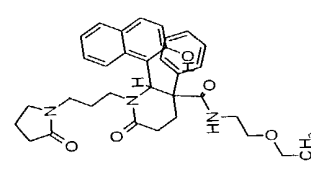
9100	2365	1	000727508	9100-033	E 07	0.34	Spy4H	51.19	0.1776	0.1776	TR0910002365	#NAME?	C <sub>27</sub> H <sub>32</sub> N <sub>2</sub> O <sub>4</sub>	448.56
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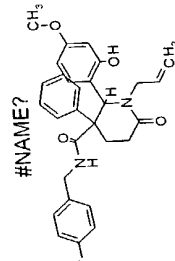
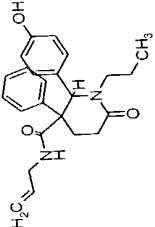
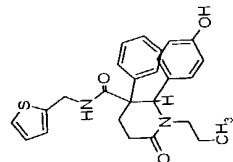
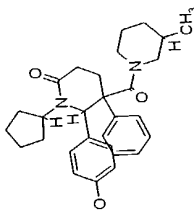


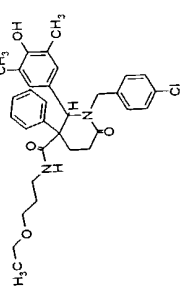
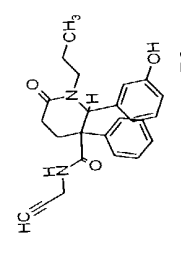
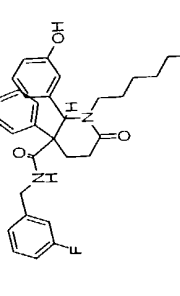
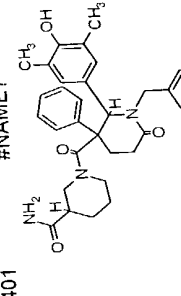
Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?		Formula	Mass
9100	588	1	000725971	9100-008	D 05	0.267	51.19	Spy4H	0.1776	TR0910000588	0.1776	TR0910000588	#NAME?		C <sub>26</sub> H <sub>34</sub> N <sub>2</sub> O <sub>4</sub>	438.563
9100	620	1	000726003	9100-008	D 09	0.264	51.19	Spy4H	0.1776	TR0910000620	0.1776	TR0910000620	#NAME?		C <sub>27</sub> H <sub>35</sub> N <sub>3</sub> O <sub>3</sub>	449.591
9100	2519	1	000727662	9100-036	G 06	0.383	51.17	Spy4H	0.1776	TR0910002519	0.1776	TR0910002519	#NAME?		C <sub>29</sub> H <sub>30</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>4</sub>	541.472
9100	1060	1	000726443	9100-014	D 04	0.269	51.06	Spy4H	0.1776	TR0910001060	0.1776	TR0910001060	#NAME?		C <sub>29</sub> H <sub>37</sub> N <sub>3</sub> O <sub>3</sub>	475.629
9100	2203	1	000727346	9100-031	C 07	0.277	51.06	Spy4H	0.1776	TR0910002203	0.1776	TR0910002203	#NAME?		C <sub>34</sub> H <sub>39</sub> N <sub>3</sub> O <sub>3</sub>	537.7

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc (mg/ml)	LionID	#NAME?		
9100	2413	1	000727556	9100-035	E 03	0.49	51.02	Spy4H	0.1776	TR0910002413		C <sub>34</sub> H <sub>33</sub> F N <sub>2</sub> O <sub>3</sub>	536.644
9100	2466	1	000727609	9100-035	B 10	0.394	51.02	Spy4H	0.1776	TR0910002466		C <sub>28</sub> H <sub>37</sub> Br N <sub>2</sub> O <sub>3</sub>	529.515
9100	965	1	000726348	9100-013	E 02	0.337	51.02	Spy4H	0.1776	TR0910000965		C <sub>30</sub> H <sub>36</sub> Br N <sub>3</sub> O <sub>4</sub>	582.535
9100	1697	1	000726840	9100-023	A 04	0.363	50.94	Spy4H	0.1776	TR0910001697		C <sub>24</sub> H <sub>29</sub> Br N <sub>2</sub> O <sub>4</sub>	489.407

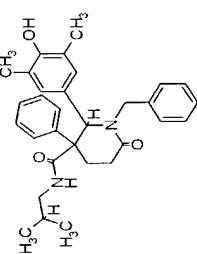
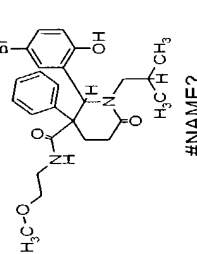
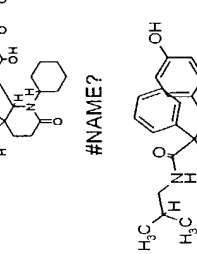
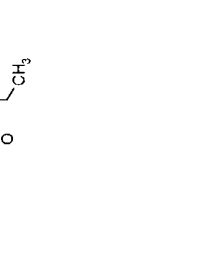
$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ -1 & i \end{pmatrix}$

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	C <sub>28</sub> H <sub>35</sub> Br N <sub>2</sub> O <sub>3</sub>	527.5
9100	1715	1	000726858	9100-023	C 06	0.557	50.94	Spy4H	0.1776	TR0910001715			
9100	3033	1	000728176	9100-042	A 11	0.445	50.94	Spy4H	0.1776	TR0910003033		496.644	
9100	3691	1	000728834	9100-051	C 03	0.457	50.92	Spy4H	0.1776	TR0910003691		524.701	
9100	3748	1	000728891	9100-051	D 10	0.275	50.92	Spy4H	0.1776	TR0910003748		557.687	

Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID		
9100	2373	1	000727516	9100-033	E 08	0.351	50.91	Spy4H	0.1776	TR0910002373		C <sub>29</sub> H <sub>29</sub> F N <sub>2</sub> O <sub>4</sub> 488.556
9100	606	1	000725989	9100-008	F 07	0.266	50.90	Spy4H	0.1776	TR0910000606		C <sub>24</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub> 392.496
9100	618	1	000726001	9100-008	B 09	0.291	50.90	Spy4H	0.1776	TR0910000618		C <sub>26</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub> S 448.584
9100	2795	1	000727938	9100-039	C 11	0.392	50.87	Spy4H	0.1776	TR0910002795		C <sub>29</sub> H <sub>36</sub> N <sub>2</sub> O <sub>3</sub> 460.614

Library	Cmpd	Lot	ExtReg	Plate	Well	Raw Data	Assay Result	Assay	Conc mg/ml	LionID	#NAME?	Chemical Structure	Molecular Formula	Mass
9100	2622	1	000727765	9100-037	F 09	0.377	50.83	Spy4H	0.1776	TR0910002622			C <sub>32</sub> H <sub>37</sub> ClN <sub>2</sub> O <sub>4</sub>	549.107
9100	1110	1	000726493	9100-014	F 10	0.272	50.78	Spy4H	0.1776	TR0910001110			C <sub>24</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub>	390.48
9100	1012	1	000726395	9100-013	D 08	0.517	50.75	Spy4H	0.1776	TR0910001012			C <sub>31</sub> H <sub>35</sub> FN <sub>2</sub> O <sub>3</sub>	502.626
9100	2401	1	000727544	9100-035	A 02	0.33	50.70	Spy4H	0.1776	TR0910002401			C <sub>33</sub> H <sub>37</sub> N <sub>3</sub> O <sub>4</sub>	539.672



Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID	#NAME?	Chemical Structure	Molecular Formula	Mass
9100	2426	1	000727569	9100-035	B 05	0.324	50.70	Spy4H	0.1776	TR0910002426	0.1776	TR0910002426	#NAME?		C <sub>31</sub> H <sub>36</sub> N <sub>2</sub> O <sub>3</sub>	484.636
9100	1687	1	000726830	9100-023	G 02	0.338	50.67	Spy4H	0.1776	TR0910001687	0.1776	TR0910001687	#NAME?		C <sub>25</sub> H <sub>31</sub> Br N <sub>2</sub> O <sub>4</sub>	503.434
9100	2342	1	000727485	9100-033	F 04	0.32	50.63	Spy4H	0.1776	TR0910002342	0.1776	TR0910002342	#NAME?		C <sub>31</sub> H <sub>42</sub> N <sub>2</sub> O <sub>5</sub>	522.682
9100	626	1	000726009	9100-008	B 10	0.284	50.62	Spy4H	0.1776	TR0910000626	0.1776	TR0910000626	#NAME?		C <sub>25</sub> H <sub>32</sub> N <sub>2</sub> O <sub>3</sub>	408.539

408.539, 522.682, 503.434, 484.636

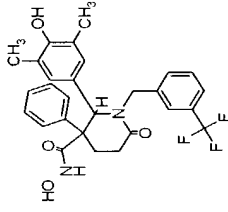


Library	Compd	Lot	ExtReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID
9100	717	1	000726100	9100-009	E 11	0.252	50.34	Spv4H	0.1776	TR0910000717		

C<sub>28</sub> H<sub>27</sub> F<sub>3</sub> N<sub>2</sub> O<sub>4</sub>

512.525

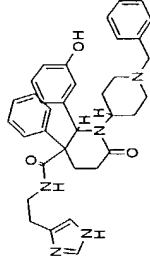
#NAME?



C<sub>35</sub> H<sub>39</sub> N<sub>5</sub> O<sub>3</sub>

577.725

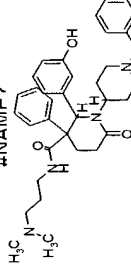
#NAME?



C<sub>35</sub> H<sub>44</sub> N<sub>4</sub> O<sub>3</sub>

568.758

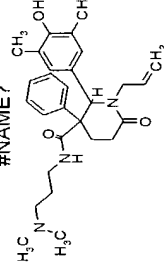
#NAME?



C<sub>28</sub> H<sub>37</sub> N<sub>3</sub> O<sub>3</sub>

463.618

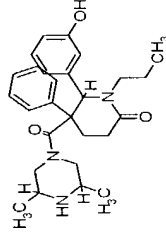
#NAME?



C<sub>27</sub> H<sub>35</sub> N<sub>3</sub> O<sub>3</sub>

449.591

#NAME?

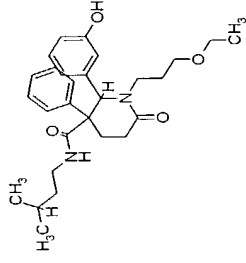


Library	Compd	Lot	ExReg	Plate	Well	Raw Data	Assay	Result	Assay	Conc	mg/ml	LionID
9100	1981	1	000727124	9100-028	E 09	0.283	50.21	Spy4H	0.1776	TR0910001981		

C<sub>28</sub> H<sub>38</sub> N<sub>2</sub> O<sub>4</sub>

#NAME?

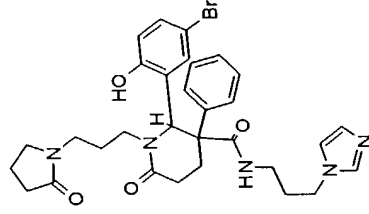
466.618



C<sub>31</sub> H<sub>35</sub> Br N<sub>5</sub> O<sub>4</sub>

#NAME?

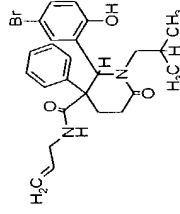
622.56



C<sub>25</sub> H<sub>25</sub> Br N<sub>2</sub> O<sub>3</sub>

#NAME?

485.419



C<sub>35</sub> H<sub>33</sub> Cl<sub>2</sub> F N<sub>2</sub> O<sub>3</sub>

#NAME?

619.561

